PNNL-17225



Microbiological, Geochemical and Hydrologic Processes Controlling Uranium Mobility: An Integrated Field-Scale Subsurface Research Challenge Site at Rifle, Colorado, Quality Assurance Project Plan

N.J. Fix

January 2008

Prepared for the U.S. Department of Energy under Contract DE-AC05-76RL01830



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Pacific Northwest National Laboratory Richland, Washington 99352

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Project # 51882

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## **Summary**

The U.S. Department of Energy (DOE) faces the challenge of cleaning up and/or monitoring large, dilute plumes contaminated by metals, such as uranium and chromium, whose mobility and solubility change with redox status. Field-scale experiments with acetate as the electron donor have stimulated metal-reducing bacteria to effectively remove uranium [U(VI)] from groundwater at the Uranium Mill Tailings Site in Rifle, Colorado. The shallow depth to groundwater (3-4 m [9.8-13.1 ft), thin saturated zone (~2.5 m [8.2 ft]), and well-defined groundwater flow system at the Rifle, Colorado, site facilitated the monitoring of microbial and geochemical processes which led to two important findings: 1) the transition from iron reduction to sulfate reduction significantly decreased the U(VI) bioreduction rate; and 2) U(VI) removal from groundwater continued for 18 months, actually increasing after acetate amendment was terminated. Understanding these behaviors in the context of site-specific hydrologic, geochemical, and biological processes and conditions is critical to the design of optimal biostimulation strategies for prolonging uranium bioremediation.

The Pacific Northwest National Laboratory and a multidisciplinary team of national laboratory and academic collaborators have embarked on a research project proposed for the Rifle, Colorado, site to gain a comprehensive and mechanistic understanding of the microbial factors and associated geochemistry controlling uranium mobility so that DOE can confidently remediate uranium plumes, as well as support stewardship of uranium-contaminated sites. Specifically, the team is testing four (4) hypotheses that address knowledge gaps in the following areas:

- 1. Geochemical and microbial controls on stimulated U(VI) bioreduction by iron-reducers
- 2. U(VI) sorption under iron-reducing conditions
- 3. Post-biostimulation U(VI) stability and removal
- 4. Rates of natural bioreduction of U(VI).

The hypotheses will be tested with a focused set of field and laboratory experiments that use recently developed sciences of proteogenomics and stable isotope probing to track microbial metabolic status and specific organisms responding to acetate amendment. The project will relate this information directly to changes in iron redox status and sulfide minerals, with field-scale changes detected by noninvasive hydrogeophysics, including three-dimensional complex resistivity tomography. The approach specifically targets new knowledge that can be translated into scientifically defensible flow and reactive transport process models of microbially mediated and abiotic reactions, taking a major step toward the DOE Environmental Remediation Science Program's long-term goal to "...incorporate coupled biological, chemical and physical processes into decision making for environmental remediation."<sup>1</sup>

<sup>&</sup>lt;sup>1</sup>Biological and Environmental Research Advisory Committee. 2004. Letter Report of the Biological and Environmental Research Advisory Committee on Long Term Performance Goals for the Office of Biological and Environmental Research. Available at <u>http://www.sc.doe.gov/ober/berac/PARTSreport.pdf</u>

This Quality Assurance Project Plan provides the quality assurance requirements and processes that will be followed by the Rifle Integrated Field-Scale Subsurface Research Challenge Project. The Quality Assurance Project Plan is based on the requirements in the *EPA Requirements for Quality Assurance Project Plans (QA-R-5)* (EPA/240/B-01/003)<sup>2</sup>; DOE Order 414.1C, "Quality Assurance"<sup>3</sup>; 10 *Code of Federal Regulations* 830, Subpart A, "Quality Assurance Requirements"<sup>4</sup>; and the *Price Anderson Amendments Act*<sup>5</sup>.

<sup>&</sup>lt;sup>2</sup> EPA/240/B-01/003 (QA/R-5). 2001. EPA Requirements for Quality Assurance Project Plans.

U.S. Environmental Protection Agency, Washington, D.C.

<sup>&</sup>lt;sup>3</sup> DOE Order 414.1C. 2005. "Quality Assurance." U.S. Department of Energy, Washington, D.C.

<sup>&</sup>lt;sup>4</sup> 10 CFR 830, Subpart A, "Quality Assurance Requirements." Code of Federal Regulations.

<sup>&</sup>lt;sup>5</sup> PAAA-Price-Anderson Amendments Act. *Energy Policy Act of 2005*. Title VI—Nuclear Matters, Subtitle A— Price-Anderson Act Amendments, Section 601 et. seq. Public Law 109-58, as amended, 42 USC 15801 et seq.

# Acronyms

| ARM    | Atmospheric Radiation Measurement Program                                |
|--------|--|
| ATS    | Assessment Tracking System   |
| BER    | Biological and Environmental Research                                    |
| CAWSRP | Conducting Analytical Work in Support of Regulatory Programs             |
| CERCLA | Comprehensive Environmental Response, Compensation, and<br>Liability Act |
| CFR    | Code of Federal Regulations  |
| CMP    | Configuration Management Plan  |
| DOE    | U.S. Department of Energy  |
| DQO    | Data Quality Objectives  |
| EPA    | U.S. Environmental Protection Agency                                     |
| ERSD   | DOE Environmental Remediation Sciences Division                          |
| ERSP   | Environmental Remediation Science Program                                |
| ES&H   | Environmental Safety and Health  |
| FREC   | Field Research Executive Committee                                       |
| FY     | fiscal year  |
| GEM    | Geospatial Environmental Mapping System                                  |
| IFC    | Integrated Field-Scale   |
| INL    | Idaho National Laboratory  |
| LBNL   | Lawrence Berkeley National Laboratory                                    |
| LM     | DOE Legacy Management Office   |
| LOI    | letter of instruction  |
| M&TE   | measuring and test equipment   |
| MDL    | method detection limits  |
| NEPA   | National Environmental Policy Act  |
| NRC    | U.S. Nuclear Regulatory Commission                                       |
| OBER   | DOE Office of Biological and Environmental Research                      |
| OJT    | on-the-job-training  |
| PAAA   | Price-Anderson Amendments Act  |
| PDF    | portable document format   |
| PI     | Principal Investigator   |
| PMP    | Project Management Plan  |
|        |  |

| DD U   |   |
|--------|---|
| PNNL   | Pacific Northwest National Laboratory               |
| PNSO   | Pacific Northwest Site Office                       |
| РО     | purchase orders                                     |
| QA     | Quality assurance                                   |
| QAP    | Quality Assurance Plan                              |
| QAPjP  | Quality Assurance Project Plan                      |
| RTDI   | Records Transfer/ Data Input Form                   |
| SBMS   | Standards-Based Management System                   |
| SC     | DOE Office of Science                               |
| SOARS  | System Operation and Analysis at Remote Sites       |
| SOW    | statements of work                                  |
| SRS    | Software Requirements Specifications                |
| UMTRA  | Uranium Mill Tailing Remediation Action             |
| UMTRCA | Uranium Mill Tailings Radiation Control Act of 1978 |
| V&VPR  | Verification and Validation Plan Review             |
| VPP    | Verification and Validation Plan                    |
| VVR    | Verification and Validation Report                  |
| WBR    | workstation backup and restore                      |
|        |   |

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## **1.0 Quality Assurance Plan Distribution**

Pacific Northwest National Laboratory (PNNL) document control will distribute this Quality Assurance Project Plan (QAPjP) internally to staff at PNNL; the U.S. Department of Energy (DOE) Office of Biological and Environmental Research (OBER); DOE Pacific Northwest Site Office (PNSO), and the DOE Legacy Management Office (DOE LM), as requested. The Project Manager will determine the final PNNL and external distribution list.

The QAPjP will also be published in accordance with the PNNL Standards-Based Management System (SBMS) subject area, "<u>Publishing Scientific and Technical Information</u>" (PNNL 2007d) and will be made available to all Integrated Field-Scale Subsurface Research Challenge Site at Rifle, Colorado (referred to as the Rifle IFC Site Project) participants as a portable document format (PDF) file via the project's SharePoint<sup>®</sup> site<sup>1</sup>.

## 2.0 Introduction

#### 2.1 Project Title

The title of this project is as follows: Microbiological, Geochemical and Hydrologic Processes Controlling Uranium Mobility: An Integrated Field-Scale Subsurface Research Challenge Site at Rifle, Colorado, Quality Assurance Project Plan.

#### 2.2 Client

The client for this project is the U.S. Department of Energy, Office of Biological and Environmental Research, Washington, D.C.

#### 2.3 Authorizing Document

This project is funded by the DOE, Environmental Remediation Sciences Division (ERSD) through the Environmental Remediation Science Program (ERSP) Notice LAB 06-16. Additional funding sources are not anticipated to be issued for the duration of the contract for this work scope. However, the QAPjP will be revised as appropriate should conditions change.

The project runs from fiscal year (FY) 2007 through FY 2011 and is projected to be funded at \$16,212,623.00. It should be noted that the first year of funding was approximately \$1,000,000.00 less than originally proposed thus the total funding for the project is likely to be less than the projected amount.

<sup>&</sup>lt;sup>1</sup> SharePoint is a registered trademark of the Microsoft Corporation.

#### 2.4 Quality Assurance Requirements

The QAPjP is based on the QA requirements of DOE Order 414.1C, "Quality Assurance," and 10 *Code of Federal Regulations* (CFR) 830, Subpart A, "Quality Assurance Requirements," as delineated in the PNNL SBMS. The QAPjP is also based on the quality assurance (QA) requirements of the *UMTRA Project Office Quality Assurance Program Plan* (DOE 1993), which required compliance with DOE Order 5700.6C, "Quality Assurance" (superseded by DOE Order 414.1C) and the *U.S. Department of Energy, Office of Legacy Management, Quality Assurance Program Plan* (DOE 2006). Field activities of the project are subject to the *Price-Anderson Amendments Act* (PAAA) compliance as defined in the PNNL PAAA Program and implemented through the SBMS subject area, "Price-Anderson Amendments <u>Act</u>" (PNNL 2007c).

#### 2.5 Special Requirements or Specifications

DOE Orders 435.1, "Radioactive Waste Management"; 5400.5, "Radiation Protection of the Public and Environment"; and 450.1, "Environmental Protection Program," apply to the project to ensure that activities related to the radioactive materials and samples are protective of human health, and fulfill PNNL's environment and stewardship requirements.

Field Experiment and Sampling and Analysis Plans (see Sections 4.0 and 5.0) will be based on the scientific method, and as appropriate, applying the Data Quality Objectives (DQO) process, in accordance with the *Guidance on Systematic Planning Using the Data Quality Objectives Process (QA/G-4)* (EPA/240/B-06/001). Field Experiment and Sampling and Analysis Plans are reviewed and approved at the project level and updated as necessary.

Computer modeling and database activities for the project shall comply with the requirements as specified in the SBMS subject areas, "<u>Safety Software</u>" (PNNL 2007f) and "<u>Software</u>" (PNNL 2007h), as appropriate. Specific safety software and software requirements for PNNL and collaborator activities are described in Section 17.0.

### 2.6 Project Scope

Surface remedial action was completed for the Rifle Processing Site in July 1996 in accordance with the *Uranium Mill Tailings Radiation Control Act of 1978* (UMTRCA) regulations as a Uranium Mill Tailing Remediation Action (UMTRA) Project. *National Environmental Policy Act* (NEPA) compliance was achieved with the October 1996 "Final Programmatic Environmental Impact Statement" for the UMTRA Ground Water Project (61 FR 67325-67326). DOE received certification from the U.S. Nuclear Regulatory Commission (NRC) for the cleanup in January 1998. NRC concurred with the Ground Water Compliance Action Plan for the UMTRA Projects Site as of July 2002. The compliance strategy selected was natural flushing for uranium in conjunction with alternate concentrations limits for vanadium and selenium. The compliance strategy of natural flushing means that selected wells will be monitored periodically by DOE LM, but no active remediation is planned. Contaminant concentrations were expected to decline slowly over the next 5 years. Site monitoring was employed to establish the background rate of changes in contaminant concentrations.

Estimating naturally occurring rates of U(VI) bioreduction is potentially of key importance to the long-term stewardship of DOE LM sites contaminated with redox-sensitive metals. Although there have

been great strides in discerning the as-yet-to-be cultured bacteria present in UMTRA samples using molecular methods, the presence and/or absence of any particular microorganism in this setting does not ensure that those bacteria are active or important in uranium reduction. This knowledge gap makes the determination of the natural (unamended) rates of uranium reduction at the Rifle site particularly hard to achieve.

The objective of the research at the Rifle site is to gain a comprehensive and mechanistic understanding of the microbial factors and associated geochemistry controlling uranium mobility at the field scale so that DOE can confidently remediate uranium plumes as well as support stewardship of uranium-contaminated sites.

The four hypotheses that form the basis of this project were developed from the current state of understanding the process, and are geared toward enabling predictable application of biostimulation for in situ removal of U(VI) from groundwater. Data obtained from the proposed experiments will be used to test the hypotheses and enable modeling of both engineered bioremediation and natural attenuation via naturally occurring microbially mediated U(IV) reduction (see modeling section below).

*Hypothesis 1*. In the presence of mM sulfate concentrations in groundwater, the transition from Fe(III) to sulfate reduction during acetate amendment will occur when the readily bioavailable Fe(III) is depleted. Iron reduction (and concomitant U(VI) reduction) can be extended in time through 1) the addition of nanoparticulate or soluble Fe(III) to the subsurface, and 2) introduction of acetate at concentrations sufficient to support iron reduction but not sulfate reduction.

*Hypothesis 2*. The sorption of U(VI) under reduced conditions is decreased overall in comparison to more oxic conditions, but is still large enough to retard U(VI) transport in the Rifle, Colorado aquifer relative to groundwater flow. Quantifying the impact of U(VI) sorption on groundwater U(VI) concentrations under iron-reducing conditions is a crucial part of numerical modeling of aquifer conditions during and after biostimulation experiments.

*Hypothesis 3.* Long-term post-biostimulation removal of U(VI) is dependent on ferrous sulfide minerals precipitated during sulfate reduction. After cessation of acetate amendment, these minerals become electron donors for a post-biostimulation microbial community capable of using low-ambient concentrations of oxygen and nitrate as terminal-electron acceptors. U(VI) is sorbed onto 1) biopolymers specific to the post-biostimulation microbial consortia, and 2) the freshly oxidized Fe(III) mineral surfaces.

*Hypothesis 4*. Slow, naturally occurring rates of microbially mediated U(VI) reduction can be estimated (low, medium, high) using molecular biomarkers in Rifle, Colorado, processing site samples by comparing the lowest acetate amendment in hypothesis 1 with samples from other Rifle site locations with no electron donor amendment.

The approach to testing these hypotheses is to conduct a suite of field and selected laboratory experiments in which input variables (such as acetate concentration) are controlled and monitoring and sampling is performed to observe the system response over a time course at selected spatial locations. For each field experiment, laboratory column experiments will be conducted before the field experiments, and detailed conceptual models will be developed into numerical models that will be used to predict and interpret experimental results. In many instances, the numerical models will include poorly constrained

parameters or processes that are not well known. Sensitivity analyses can be used to determine which of these are important to system behavior, thus providing the basis for improved experimental designs over time. Identification of these areas of process and parameter uncertainty is critical for developing a thorough predictive capability for contaminant transformation and translocation at DOE sites. Models will be initially calibrated against the outcome of the column experiments, and the proposed research will provide new insights into the scaling of such results via modeling from the laboratory to the field. Selected biostimulation column experiments will be conducted for longer time periods than are practical in the field, and combined with the in situ experiments and simulation, will give insights into long-term biostimulation schemes at a field site.

Table 2.1 lists field and laboratory experiments planned for this project from 2007 to 2011. This schedule is from the original project proposal and has already been modified as result of a co-Principal Investigator and collaborator meeting to initiate the project. Basically, the decision was made to conduct an initial "F-0" experiment in FY 2007.

**Note:** Appendix D contains a more detailed schedule for FY 2007 and 1 month of FY 2008. The detailed project schedule will be updated frequently and made available to project participants as PDFs on the project's SharePoint site.

| Hypotheses/Experiment   |   | Y 2    | 007 | ' | F | Y 2 | 008 | } | F | Y 2 | 009 | ) | F | Y 2 | 01( | ) | F      | Y 2 | 011 |   |
|---|---|--------|-----|---|---|-----|-----|---|---|-----|-----|---|---|-----|-----|---|--------|-----|-----|---|
| Year →  | Y | Year 1 |     |   |   | ear | 2   |   | Y | ear | • 3 |   | Y | ear | 4   |   | Year 5 |     |     |   |
| Quarter →   | 1 | 2      | 3   | 4 | 1 | 2   | 3   | 4 | 1 | 2   | 3   | 4 | 1 | 2   | 3   | 4 | 1      | 2   | 3   | 4 |
| Hypothesis 1  |   |        |     |   |   |     |     |   |   |     |     |   |   |     |     |   |        |     |     |   |
| L-1-A. Characterizing the transition from iron- to sulfate-<br>reduction under ambient conditions                                       |   |        |     |   |   |     |     |   |   |     |     |   |   |     |     |   |        |     |     |   |
| L-1-B. Maintenance of iron-reducing conditions via acetate-<br>limitation   |   |        |     |   |   |     |     |   |   |     |     |   |   |     |     |   |        |     |     |   |
| F-3. Biostimulation with low-acetate concentrations, tracking the duration of iron reduction  |   |        |     |   |   |     | V   |   |   |     | ▼   |   |   |     |     |   |        |     |     |   |
| L-1-C. Maintenance of iron-reducing conditions via ferric iron amendment  |   |        |     |   |   |     |     |   |   |     |     |   | V |     |     |   |        |     |     |   |
| F-5. Biostimulation with low acetate concentrations, followed by increased acetate and then Fe(III) amendment                           |   |        |     |   |   |     |     |   |   |     | ▼   |   |   |     | V   |   |        |     |     |   |
| L-1-D. Recovery of system poised at sulfate-reduction through modified electron donor (acetate) or acceptor (ferric iron) amendment     |   |        |     |   |   |     |     |   |   |     |     | ▼ |   |     |     |   |        |     |     |   |
| F-9. Optimal electron donor and/or receptor amendment under high DO conditions. (Test of proteomic and modeling predictive capability.) |   |        |     |   |   |     |     |   |   |     |     |   |   |     |     |   |        |     |     | V |
| Hypothesis 2  |   |        |     |   |   |     |     |   |   |     |     |   |   |     |     |   |        |     |     |   |
| L-2-!. U(VI) Sorption under baseline Rifle <sup>a</sup> conditions  |   |        |     | V |   |     |     |   |   |     |     |   |   |     |     |   |        |     |     |   |
| L-2-B. Abiotic effect of sorbed ferrous ion on U(VI) sorption   |   |        |     |   |   | V   |     |   |   |     |     |   |   |     |     |   |        |     |     |   |
| F-4. Tracer test with accelerated U(VI) desorption  |   |        |     |   |   |     |     | V |   |     |     |   |   |     |     |   |        | ▼   |     |   |
| L-2-C. U(VI) Sorption on bioreduced Rifle <sup>a</sup> sediments  |   |        |     |   |   |     |     |   | V |     |     |   |   |     |     |   |        |     |     |   |
| L-2-D. Acceleration of U(VI) desorption from contaminated   |   |        |     |   |   |     |     |   |   |     |     |   |   |     |     |   |        |     |     |   |
| Rifle <sup>a</sup> sediments  |   |        |     |   |   |     |     |   |   | •   |     |   |   |     | -   |   |        |     |     |   |
| F-6. Tracer test under reducing conditions without biostimulation   |   |        |     |   |   |     |     |   |   |     |     |   |   | V   |     |   |        |     |     |   |
| F-8. Combined biostimulation/sorption experiment. (hypotheses 1 and 2)  |   |        |     |   |   |     |     |   |   |     |     |   |   |     |     |   |        |     | ▼   |   |

Table 2.1. Planned Field and Laboratory Experiments, 2007 – 2011

| Hypotheses/Experiment   |   | FY 2007 |                                 |        |   | FY 2008 |   |   |        | FY 2009 |   |   |        | Y 2 | 010 | FY 2011 |   |        |     |  |
|---|---|---------|---------------------------------|--------|---|---------|---|---|--------|---------|---|---|--------|-----|-----|---------|---|--------|-----|--|
| Year →  |   |         |                                 | Year 1 |   |         |   |   | Year 3 |         |   |   | Year 4 |     |     |         |   | Year 5 |     |  |
| Quarter →   | 1 | 2       | 3                               | 4      | 1 | 2       | 3 | 4 | 1      | 2       | 3 | 4 | 1      | 2   | 3   | 4       | 1 | 2      | 3 4 |  |
| Hypothesis 3  |   |         |                                 |        |   |         |   |   |        |         |   |   |        |     |     |         |   |        |     |  |
| L-3-A. Biostimulation column experiments with a range of sulfate concentrations to assess relative importance of biopolymer versus abiotic FeS oxidation on sorption surfaces |   |         |                                 |        |   |         |   |   |        |         |   |   |        |     |     |         |   | ▼      |     |  |
| F-7. Biostimulation with low acetate concentration and/or ferric iron amendment, driven to sulfate reduction, with extensive sampling post-biostimulation for ~2 years        |   |         |                                 |        |   |         |   |   |        |         |   |   |        |     |     |         | ▼ |        |     |  |
| Hypothesis 4  |   |         |                                 |        |   |         |   |   |        |         |   |   |        |     |     |         |   |        |     |  |
| F-1. Bi-monthly sampling of background wells in years 1-3 for protein expression, gene expression, PLFA and TRFLP   |   |         |                                 |        |   |         |   |   |        |         |   |   |        |     |     |         |   |        |     |  |
| F-2. Deployment of in situ sediment incubators in background areas; initial conditions in the incubator both sterile and biostimulated  |   |         |                                 |        |   |         |   |   |        |         |   |   |        |     |     |         |   |        |     |  |
| <sup>a</sup> Rifle IFC Site.<br>▼ = Publication milestone.  |   |         | Lab Experiment Field Experiment |        |   |         |   |   |        |         |   |   |        |     |     |         |   |        |     |  |

A key element of the approach is to perform selected, focused column experiments, mostly conducted before field experiments. For the biostimulation laboratory experiments, microbiology, proteomic, geochemistry, and geophysics data will be collected systematically such that coherent data sets are available for assessing relationships among key parameters before conducting related field experiments.

The principal method to coordinate diverse disciplines on the project is to use laboratory studies and field experiments as the integrating project activity. Because data collected during experiments cannot readily be interpreted independently, participants need to connect to accomplish the experimental and project objectives. To foster this, the lead Principal Investigator (PI) will assign co-PIs to working groups for each experiment with the responsibility of interpreting and publishing results. Coordination will also be facilitated by 1) using a website presenting both real time and weekly updates of field and column experimental data, and 2) conducting monthly teleconferences with co-PIs to discuss current data collection status and interpretations. Finally, reactive transport modeling will serve as the overarching integrator. The experimentalists working on the project are expected to frame their data to support a quantitatively predictive understanding of field-scale uranium bioremediation. On the other side, modelers support experimental design and sampling plans for hypothesis testing that lead to the identification and parameterization of mechanistic process models.

The data management task will implement a central, web-accessible database, which will enable remote collaborative efforts. Users will be able to view all samples, characterization measurements, and experimental data. Raw data, sampling metadata, and instrument calibration will be stored to allow an auditable, reproducible link between field measurements and finalized data. Rigorous, workflow-based processes will be established to link field data to numerical predictive models to allow reproducibility. The model for a project website is the "Science" tab of the Atmospheric Radiation Measurement (ARM) Program website (<u>http://www.arm.gov/science/key.stm</u>), which covers the past, ongoing, and planned ARM experiments. For the Rifle IFC Site Project, website capabilities are anticipated to foster integration of diverse project activities. For project participants a password-protected website will be available to ensure that unauthorized access is not permitted. A public website will include selected real-time data streams for educational purposes and to increase the visibility of the project and broaden interest

by the scientific community. The same network will support an electronic notebook and the deployment of temporary monitoring stations. Key elements of this approach include the following:

- *A centrally managed data repository.* This repository will consist of a number of either relational databases or spreadsheets that will house all data (geochemical, hydrological, geophysical, microbiological, environmental and experimental) collected as part of the Rifle IFC Site Project. These databases will contain information on sensors, analytical procedures, and instruments consisting of the raw data and calibration equations used. The repository will also contain modeling results.
- *A web interface providing access.* This web interface will allow data access in a tiered manner. This will allow IFC scientists to publish and analyze results from ongoing experiments prior to data becoming publicly accessible. Eventually, the web interface will also include tools for basic data processing and visualization (e.g., statistical analyses, time-series graphing, data contouring and three-dimensional visualization). This will be implemented through a scientific workflow system.
- *Inventories of solid and liquid samples available to other investigators.* A critical aspect of the Rifle IFC Site Project research is providing access and highly valuable samples to other ERSD investigators. The availability of such samples, their analytical characteristics, and other research results generated on them will be readily traceable and linked through the website interface and associated sample database or lists.
- *Integration of additional data sources*. Ongoing regulatory-driven data acquisition at the Rifle UMTRA site has resulted in a considerable amount of data that will be used in the overall analyses of experiments performed by the Rifle IFC Site Project. These data are contained in databases that will be accessed via links from the Rifle IFC Site Project data management system.

The Rifle IFC Site Project will develop appreciable subsurface characterization data on the hydrogeology, microbiology, and geochemistry of the field experimental domain; and field results from the experimental evaluation of hypotheses 1-4. These results will be further complemented with laboratory studies that seek to optimize experimental conditions for the field experiments. All of these results and other relevant experimental and procedural information will be captured in the data management system, making them readily accessible to project team members and other ERSD investigators as they are published.

The Interpretational Program will have three primary objectives:

- 1. Develop conceptual and numeric geohydrologic, geochemical/biogeochemical, and microbiologic models of the Rifle IFC Site
- 2. Develop, if necessary, new, alternative, or otherwise different mass-transfer models that couple with hydrologic, geochemical, or microbiological processes
- 3. Use these resulting conceptual and numeric models for field experiment evaluation and hypothesis resolution using a variety of mathematical, geostatistical, and other modeling approaches practiced by the project team members. The project will support the STOMP computational model as its primary, multiprocess integrative model.

The current capabilities of STOMP are well-suited to the range of analyses and experiments proposed by this project: characterization of processes and properties, experimental design and interpretation, testing hypotheses and alternative conceptual models, and prediction. Code modifications are anticipated to address specialized routines for biogeochemistry and mass transfer; however, these are considered to be minor changes to existing capabilities.

Management processes, including planning, scheduling/execution, and providing resources for work to prepare project deliverables based on risk, safety, life cycle, and complexity are described in the *Microbiological, Geochemical and Hydrologic Processes Controlling Uranium Mobility: An Integrated Field-Scale Subsurface Research Challenge Site at Rifle, Colorado Project Management Plan* (Project No. 51882, current revision).

The scope of this QAPjP is to provide PNNL project staff and collaborators with the program-specific planning, execution, assessment of work, and controls necessary to provide products/solutions and services of the highest quality consistent with project risks, PNNL SBMS "<u>Policies and Standards</u>" (PNNL 2006b) and the needs, expectations, and resources of the client.

### 2.7 Change Control (Scope, Schedule, Budget)

The project scope, schedule, and budget baseline are compiled, tracked, and reported using a project control system in accordance with DOE direction.

Changes in work scope, schedule, or budget may be necessary during the year. For those activities under the control of PNNL, changes may be requested of subcontractors and collaborators by PNNL that will result in a change to the statements of work (SOWs) due to revisions of work scope, schedule, and/or budget. These changes will be documented in revisions or addenda to the existing SOWs and a PNNL Subcontract Supplement Form shall be completed.

Administrative changes requested of subcontractors and collaborators approved by the Project Manager may be authorized via verbal or electronic messages. Written documentation of the changes provided verbally or in electronic messages should be maintained in the permanent project files. These changes may only be made if technical work scope and budget are not significantly affected.

## 3.0 Project Organization and Responsibilities

Research at the site will be coordinated and managed by PNNL and the DOE Grand Junction LM Office with oversight by the DOE Office of Science (SC) Biological and Environmental Research (BER) Field Site Coordinator. Decision-making authority for science activities, including final authorization to start field campaigns, will rest with PNNL via the Principal Investigator in consultation with the co-Principal Investigators. Daily execution of field experiments will be the responsibility of the Experimental Co-Principle Investigator the Field Site Manager, and staff. Routine sampling and sample analysis will be performed by the Field Site Manager's staff. However, the management approach and funding allocation assumes that co-Principal Investigators will participate in field experiments for which they are responsible by employing appropriate staff (Rifle, Colorado, graduate students or postdocs) for experiment work to ensure that sophisticated sampling and monitoring approaches are conducted at the highest level of quality. Specific roles are provided below. The coordination and management approach is designed to ensure quality experimental outcomes while maintaining safe operations.

The coordination and management approach is designed to ensure quality experimental outcomes while maintaining safe operations. The principal management mechanism will be specific, detailed experimental plans for each field experiment. These plans must be consistent with safety, training, NEPA, and regulatory requirements and will receive extensive independent review for overall scientific approach, technical details, and health and safety. Field experimental plan review will involve independent experts convened by DOE SC, the DOE (SC and LM), regulators, City of Rifle, Colorado, officials, and a local community representative, when appropriate. The reviews will be conducted on an as-needed basis using telephone conferencing or videoconferencing to minimize travel costs. Major experimental work will be done at the site only after review and approval (by the DOE SC BER Field Site Coordinator) of the governing experimental plan. The Principal Investigator or the responsible co-Principal Investigator shall be on site at the start of an experiment to ensure that the technical preparation for the experiment meets or exceeds the experimental and environmental, safety and health (ES&H) objectives outlined in the approved test plan. Field safety, NEPA, and regulatory compliance shall be the responsibility of the Field Site Manager.

Line authority, quality assurance authority and support within PNNL, and client interfaces are shown organizationally in Figure 3.1. The responsibilities of key personnel are summarized in Section 3.1. Changes to organizational/interface structures shown in Figure 3.1 that do not reflect a change in the overall scope of the activities or a change of requirements will not require a QAPjP revision and will be incorporated into the next required revision of the QAPjP.

## 3.1 Responsibilities of Key Personnel

- **Project Manager** Responsible for development and implementation of the project management plan, health and safety plan, and QAPjP. Serves as the primary-client interface to assure that customer expectations for quality, cost, and schedule are met. Provides overall direction to task managers and project personnel within PNNL to accomplish project objectives; coordinates and executes project controls associated with scope, schedule, and budget baselines; reports on project status; assures that the project is staffed with technically qualified personnel; and assures the QAPjP is implemented.
- **Task Leaders** Oversees task-specific planning, control, communications, and progress reporting; prepares scope, resource needs, cost baseline, and deliverables; assures quality and timeliness of the work in accordance with plans, policies, and procedures; provides monthly reports; and interfaces with DOE, other contractors, subcontractors, and other Task Leaders.
- **Principle Investigators** Provides task-specific technical plans, communications, and progress reporting to the Task Leader; prepares technical details of the task plan; assures technical quality of the work; supports the Task Leader to assure work is performed on schedule, within budget, and in accordance with plans, policies, and procedures; assigns and directs work of project staff; interfaces with DOE, other contractors, subcontractors, and other investigators.



Figure 3.1. Project Interfaces

- **Project Quality Engineer** Provides guidance and direction to Project Manager, Task Leads, and project staff within PNNL on PNNL QA Program requirements; performs assessments to assure quality of the work; develops, updates, and approves the QAPjP; and reviews and approves appropriate work plans and procedures.
- Other Project Staff Assures technical quality of the work and that it is performed on schedule, within budget, and in accordance with plans, policies, and procedures; and reports concerns, such as unsafe conditions, and stops work as necessary.

## 3.2 Other Work Services

Other work services for various portions of project work will be through the purchasing process. General work scope, work requirements, specifications, and QA requirements are communicated via a contracting mechanism to various subcontractors (see Section 15.0). This project is funded as pure science and research by the DOE OBER; however, one of the goals of the project is to transfer impactful science and models from the Rifle IFC Site Project to the remediation program for the DOE complex during and immediately after project completion. This information may be used in the selection of technologies for the remediation of *Comprehensive Environmental Response, Compensation, and Liability Act* (CERCLA) operable units. Therefore, SOWs and test plans used for groundwater and sediment sampling and analysis will require compliance with the *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA/240/B-01/003), and will specify requirements to be achieved by appropriate quality documents. SOWs will include instructions for inspecting supplies and consumables used for this project, as appropriate.

Subcontracts for drilling, sediment sampling, groundwater sampling, and associated support activities will include the following:

- S.M. Stoller performs routine groundwater sampling and water-level measurements as directed, purge water containment and disposal (when required), radiological control technician support, and miscellaneous solid-waste disposal.
- S.M. Stoller also provides drilling, sediment and water sample collection related to drilling, and well construction services.
- Other subcontractors may provide civil surveys, special analytical services, or other services.

Other work services for various portions of project work will be through the purchasing process. General work scope, work requirements, specifications, and QA requirements are communicated via a contracting mechanism to various subcontractors (see Section 15.0).

Contracted services received from S.M. Stoller or other Rifle IFC Site Project contractors may include construction of fences and enclosures, onsite laboratory trailers, surveying, etc.

Project staff will perform sampling and measurements according to written and approved internal procedures or test instructions. Analytical activities conducted by the project staff shall be conducted in accordance with written procedures or test instructions. Field measurements and the conduct of project

field activities will be conducted in accordance with in-house operating procedures. Project staff members are responsible for preparing data reports that summarize the results of analyses, quality control data for the method used, and identification of data qualifiers. The results and raw data will be included in the project records.

#### 3.2.1 Analytical Services

The analytical laboratories onsite, and at other DOE national laboratories are responsible for preparing data reports that summarize the results of analyses and detailed data packages that include the following:

- Sample receipt and tracking documentation, including identification of the organization and individuals performing the analysis; names and signatures of the responsible analysts; sample-holding time requirements; references to applicable chain-of-custody procedures; and dates of sample receipt, extraction (if applicable), and analysis.
- Quality control data, as appropriate for the methods used, including (as applicable) matrix spike/matrix spike duplicate data, recovery percentages, precision and accuracy data, laboratory blank data, and identification of any nonconformance that may have affected the laboratory's measurement system during the time period in which the analysis was performed.
- Analytical results or data deliverables, including reduced data and identification of data qualifiers and contractually defined reporting comments.

These requirements, as well as QA and technical requirements, are specified in the SOW to the analytical laboratories or by reference to this document. Also, the requirements for the hard copy and/or electronic data received from the analytical laboratories are specified in respective analytical subcontractor SOW.

#### 3.2.2 Sampling Services

The individual or organization performing sampling is responsible for 1) obtaining the samples; 2) delivering samples to the laboratory; and 3) delivering completed paperwork to PNNL to implement sample tracking. All activities associated with the sample collection, sample handling, sample labeling, and custody of the samples in the field shall be consistent with the recommendations and protocol provided in Chapter 4, Section 4.2 through 4.4 in *RCRA Ground Water Monitoring Technical Enforcement Guidance Document* (National Water Well Association 1986), *Test Methods for Evaluating Solid Waste, SW-846 Third Edition* (EPA/SW-846, as amended), and the *Handbook for Analytical Quality Control in Water and Wastewater Laboratories* (EPA-600/4-79/019). Activities associated with the sample collection, sample handling, sample labeling, and custody of the samples in the field shall be consistent with the SOW.

#### 3.2.3 Well Drilling, Sampling, and Construction Services

S.M. Stoller provides well-drilling and construction subcontractors and oversight for the Rifle Site. S.M. Stoller is responsible for 1) well-drilling design specifications and contract management, 2) site preparation and documentation requirements, 3) sediment and water sample collection during drilling (if required), 4) supporting hydrologic tests conducted during drilling (if required), and 5) well construction and development. Well construction will meet the requirements of 2 CCR 402-2. Well drilling and construction, sediment and water sampling, testing support, and associated quality requirements will be specified in the SOW to S.M. Stoller or by reference to this document. S.M. Stoller may subcontract work activities provided the requirements in the SOW and the S.M. Stoller QA Program are met by subcontractor(s).

#### **3.2.4** Geophysical Subsurface

Lawrence Berkeley National Laboratory (LBNL) is responsible for conducting surface geophysics and geophysical logging in Rifle IFC Project site wells on the site. PNNL provides technical support to LBNL to ensure that the geophysical logging requirements and associated quality requirements are met. Requirements for data deliverables are also specified in the SOW.

Other geophysical subsurface activities are provided by LBNL and other collaborators on the project as needed. LBNL and/or the collaborators are responsible for obtaining these geophysical services. LBNL provides technical support to the collaborators to ensure geophysical logging requirements and associated quality requirements and data deliverables are specified in the SOW to the proposed subcontractor.

#### 3.2.5 Field Measurements

Field measurements during well drilling will be conducted in accordance with Stoller Corporation procedures during well drilling or other equivalent procedures, and as directed in the SOW. Specific project-reviewed and -approved test plans will address procedures during field experiments.

#### **3.2.6** Other Services

Other subcontracted services received from Stoller Corporation or other Rifle site contractors may include construction of fences and enclosures, onsite laboratory trailers, etc.

### **3.3** Work Conducted by Project Staff

Analytical activities conducted by project staff in support of the Rifle IFC Site Project shall be conducted in accordance with written standard operating procedures documented in test plans associated with experiments, as appropriate. Field measurements will be conducted in accordance with in-house operating procedures or contractor procedures, as appropriate. The project staff members are responsible for preparing data reports that summarize the results of analyses, quality control data for the method used, and identification of data qualifiers. The results and raw data will be included in the project records.

Project staff will perform sampling and measurements according to written and approved test plans (Section 5.1), written procedures, or other written direction.

#### 3.4 Field Work

Field work is executed by Rifle IFC Site Project staff. Prior to executing field work, project-specific test plans are developed, as described in Section 5.0. If supplemental information or individual parameters are needed to perform a test, a test instruction will be developed. The test instructions and test

plans shall be reviewed by a technical reviewer and project Quality Engineer as determined through consultation between the Quality Engineer and the Project Manager.

## 4.0 Data Quality Objectives

The QA objectives for measurements generally applicable to technology investigations under the purview of this QAPiP are primarily related to the following: 1) the definition of appropriate methods and analytical precision and accuracy appropriate for chemical analysis of the analytes of interest; and 2) the definition of methods and limits and values for physical measurements associated with the investigation (e.g., column tests). Discussions of aqueous sample analytical objectives and analytical methods with corresponding target values for detection limits, precision, and accuracy are provided in Appendix A of this QAPjP; the Environmental Sciences Laboratory OA Plan (QA ESL, current revision); individual test plans; and test instructions and/or test procedures. The sediment analytical objectives and analytical methods with corresponding target values for detection limits, precision, and accuracy are provided in the Environmental Sciences Laboratory OA Plan (QA ESL), individual test plans, and/or test procedures. Where appropriate, DQOs were developed in accordance with Guidance on Systematic Planning Using the Data Quality Objectives Process (QA/G-4) (EPA/240/B-06/001) will be applied. Other measurement objectives and methods with corresponding target values for detection limits, precision, and accuracy (as applicable) are provided in the specific work plans and/or the SOW for such activities. Specific data quality needs for individual investigations that are different than the requirements established herein shall be addressed within individual work plans. Other measurement considerations, accuracy requirements, units, and data recording and reporting protocols for instruments supporting stratigraphic characterization, aguifer testing, and other types of field investigations shall be as specified in the applicable plans and/or procedures. Because of the dynamic nature of many of the field experiments conducted, some field measurements, samples, and tests are conducted in response to unpredicted test conditions. Under these circumstances, special measurements and samples will be documented as performed.

### 5.0 Test Plans and Procedures

Test plans and procedures are used to assure that activities affecting quality are performed consistently and correctly. Test plans are prepared by project staff to conduct a single experiment or test as identified below. In particular, detailed experimental plans shall be prepared for each field experiment. These plans must be consistent with safety, training, NEPA, and regulatory requirements and will receive independent review for overall scientific approach, technical details, and health and safety. Field experimental plan reviews shall involve independent experts convened by DOE SC. Regulators will review plans as appropriate, and City of Rifle, Colorado, officials and a local community representative will be provided plans in advance of conducting tests. Reviews will be conducted on an as-needed basis using videoconferencing and/or e-mail to minimize travel costs. Major experimental work shall be done at the site only after review and approval by the DOE SC BER Field Site Coordinator.

Because linking laboratory experiments to field experiments is such an important part of this project, experimental plans shall be required for the proposed laboratory experiments. While these plans are

expected to be less detailed than field plans, they will be reviewed and approved by the Principal Investigators, co-Principal Investigators, and an appropriate laboratory safety officer in the performing institution. Leading environmental researchers throughout the country will be informed of the availability of groundwater, sediment, and other samples from the Rifle, Colorado, site for research purposes by 1) presentations given at national meetings hosted by the American Society for Microbiology, American Geophysical Union, Geological Society of America, and the American Chemical Society; 2) an article or announcement in at least two news publications of those same organizations; and 3) a website with a section detailing the protocols for obtaining groundwater, sediment, and other samples. Access to samples will be accorded to project and non-project researchers alike, as deemed appropriate by the Principal Investigator.

## 5.1 Test Planning and Performance

Test plans will be used to document a single or related set of experiments or tests (e.g., hydrologic field tests, or vertical sampling) work activity.

### 5.1.1 Developing the Test Plan

The test plan shall contain the following information:

- A title and/or number including date or revision.
- Dated signatures of the Preparer, Technical Lead, Project Manager or Task Lead, and Quality Representative.
- Individual page identification (page \_\_\_\_ of \_\_\_\_).

The content of each test plan will depend on the scope of the test. The following is a brief description of mandatory and optional items to be considered in the preparation of the test plan:

• **Purpose/Description (mandatory)** – Provide a short narrative on the purpose of the experiment, test, or activity.

*Example:* The purpose of this test is to provide hydrologic property data at polyphosphate treatability injection test wells.

• **Prerequisites (mandatory)** – List items, conditions, or other concerns that must be satisfied prior to beginning the test.

*Example:* Prior to beginning the work activity, the staff must complete special training on other plans or procedures that will be used in conjunction with the test plan, special handling or storage requirements, special access or permits, and required records that need to be generated as the result of the work activity.

• Safety (mandatory) – Describe the hazards associated with the work such as physical agents (e.g., temperature, pressure, noise, electrical); hazardous environments (e.g., confined spaces, remote locations, heat/cold stress); and hazardous materials (e.g., flammables, corrosives, highly toxic,

carcinogens). Describe the methods used to mitigate the hazards that were identified (e.g., personal protective equipment, time periods away from the hazard, alarms, location of nearest aid station).

- Materials and Equipment (optional) List the materials and equipment that are necessary to complete the work.
- Measuring and Test Equipment (mandatory) List the equipment that will be used to make the measurements; include the calibration requirements, system checks, and quality control checks in this section or in the work instructions section of the test plan.
- Pretest Verification (mandatory) Determine if certain items of a test require verification prior to their use and indicate how the verification will be done.

*Example:* A tracer solution containing Br will be used throughout the test and the initial concentration shall be known. The solution shall be measured by the calibrated probe (as described above) and the concentration shall be recorded prior to injection.

- **Documentation and Reporting (mandatory)** Describe where the data collected during the test should be documented (e.g., field record forms, laboratory record books [LRBs], entered into a computer, downloaded from computer to hardcopy). Additionally, describe what will be reported, to whom, and the due date(s).
- Work Instructions (mandatory) Provide step-by-step instructions and/or nonsequential instructions (whichever is more appropriate to the activity). Each step or instruction shall be as simple as possible but with sufficient detail so that individuals experienced in the technology or activity involved can easily understand. The following types of information should be considered for inclusion: administrative control hold points (i.e., where safety, quality, radiological, or other approvals or actions are required before proceeding); cautions that indicate potentially hazardous situations which, if not avoided, may result in death, injury, or damage to facilities or equipment; and notes that call attention to supplemental information that assist the user in making decisions or improving work performance.

#### 5.1.2 Test Performance

Tests will be performed in accordance with the test plans, which shall be available at the work location. The Technical Lead is responsible for assuring that the current version is used to perform the work.

If changes to the test plan are required during the execution of the work, the Technical Lead shall document the deviation, and the justification or rationale for the change.

### 5.2 Procedures

Procedures will be developed in accordance with the SBMS subject area, "<u>Procedures, Permits, and</u> <u>Other Work Instructions</u>" (PNNL 2004). Project staff will perform scheduling, data verification, data processing, and data management as described in Section 6.0 and by following the applicable internal technical procedures or instructions.

#### 5.2.1 **Project Procedures**

Procedures used by PNNL project staff will be developed in accordance with the SBMS subject area, "<u>Procedures, Permits, and Other Work Instructions</u>" (PNNL 2004). Project staff will perform scheduling, data verification, data processing, and data management as described in Section 6.0 and by following the applicable internal technical procedures or instructions. Also, project staff will perform groundwater sampling, field measurements, water-level measurements, and aquifer testing by following the appropriate Rifle Site technical procedures.

#### 5.2.2 Calibration Procedures

Requirements for calibrating field and analytical laboratory instruments and maintaining traceability to national or international standard (e.g., National Institute of Standards and Technology) is in accordance with *Test Methods for Evaluating Solid Waste: Physical/Chemical Methods, SW-846, Third Edition* (EPA/SW-846, as amended). These requirements are passed to the subcontractors by a SOW. PNNL will periodically assess the use and effectiveness of procedures and systems for calibration of equipment with the subcontractors.

Measuring and test equipment (M&TE) used by PNNL staff to collect quality-affecting data that are calibrated by the user (Category 2 M&TE) or by an approved external or internal source (Category 1 M&TE) will be in accordance with the SBMS subject area, "<u>Calibration</u>" (PNNL 2005b). Upon receiving calibrated equipment, staff must review the documentation for acceptability, verify the proper operation of the M&TE, and check the calibration label.

M&TE shall be controlled in accordance with the SBMS subject area, "<u>Calibration</u>" (PNNL 2005b). Externally calibrated M&TE, such as balances, will be calibrated in accordance with manufacturers' tolerances unless other control limits are specified and justification is provided.

Data sheets and log-book entries will be used to document pipette performance checks. Calibration reports and other calibration data will be maintained as project records.

Quality control requirements are described in Appendix A of this QAPjP. A few exceptions to these requirements are considered necessary for the project, as described in the following paragraphs.

#### 5.2.3 Common Data Quality Calculations

Data quality parameters of precision, accuracy, measures of agreement, detection limits/sensitivity, and uncertainty will be calculated per the formulas in CAWSRP, Section 6, in the exhibit "Calculations for Assessing Data Quality." For radiochemistry analyses, the minimum detectable activity (MDA) is reported as the detection limit.

Control charting is a tool used to monitor an ongoing/continuous process where there are sufficient data points to perform a representative statistical evaluation. The analyses performed within this project are performed as a research function in which instrumental operating parameters may be changed to accomplish many different objectives. The frequency of instrumental operating changes does not allow accumulation of sufficient data points to properly use control charting as a statistical analysis tool. In lieu of control charts, instrument performance is monitored daily by the use of fixed control limits.

#### 5.2.4 Water-Level Procedures

Procedures for water-level measurements shall be written in accordance with industry accepted standards, such as guidelines prepared by the U.S. Geological Survey (1977), and updated as required for the latest advances in measuring equipment.

#### 5.2.5 Analytical Procedures

The specific work plans and/or test plans identify the constituents to be analyzed. As applicable, a PNNL internal procedure generates the sampling package (e.g., chain-of-custody form), which identifies the analytical methods, sample identification, and other data on the chain-of-custody form. The chain-of-custody form and samples are provided to the appropriate analytical laboratory. Administrative quality assurance processes and procedures (e.g., chain-of-custody, custody logs, sample handling, storage and disposal, training) will be required of the onsite and offsite analytical laboratories and will be specified in the SOW. The analytical methods required may be contained within the following references:

- Test Methods for Evaluating Solid Waste: Physical/Chemical Methods, SW-846, Third Edition (EPA/SW-846, as amended)
- Methods for Chemical Analysis of Water and Wastes (EPA-600/4-79-020)
- Methods for the Determination of Organic Compounds in Drinking Water (EPA-600/4-88-039)
- Prescribed Procedures for Measurement of Radioactivity in Drinking Water (EPA-600/4-80-032)
- Procedures for Radiochemical Analysis of Nuclear Reactor Aqueous Solutions (EPA-R4-73-014)
- Radiochemical Analytical Procedures for Analysis of Environmental Samples (EMSL-LV-0539-17).

Many radiochemical methods have not been standardized, but the procedures are documented in the laboratory specific-standard operating procedures. Aqueous sample chemical and radiological analytical methods and requirements for constituents are specified by the SOW, work plan, or other written direction. Similarly, microbiological analytical methods may be developed based on initial response of samples and so may be difficult to specify in advance. In these cases, the protocols and procedures are developed and documented as work progresses.

Most potential chemical constituents to be analyzed are provided in Appendix A, Table A.3 of this QAPjP and/or the *Environmental Sciences Laboratory QA Plan* (QAP ESL, current revision). Sediment and other media constituents to be analyzed and corresponding analytical methods and procedures will be passed on to the analytical laboratory by a SOW, work plan, or other written direction.

Method detection limits (MDLs) shall be determined for all nonradiochemical methods required by the project. Water MDLs shall be determined in accordance with 40 CFR 136, Appendix B, "Definition

and Procedure for the Determination of the Method Detection Limit—Revision 1.1." The laboratory provides MDL studies results to PNNL as specified in the SOW. Required detection limits for radiochemical methods are provided in the SOW, work plan, or other written direction.

Sediment constituents to be analyzed for, as well as the corresponding analytical methods and procedures, will be passed on to the analytical laboratory by a SOW. The MDLs for sediment analysis shall be determined using the calculation provided in Chapter One of EPA/SW-846, as amended.

Technical procedures not previously documented will be developed and used as described in Appendix C. If supplemental information or individual parameters are needed to perform a test, a test instruction will be developed. The test instruction shall be reviewed by a technical reviewer and must include the following information:

- A unique numerical designation
- Revision number
- Title
- Effective date
- Instructions operating parameters and specific test run information such as sample size and/or composition, temperature, pH, test duration, etc.
- Reference to controlling procedure or test plan
- Approval by author
- When well-established methods (e.g., American Society for Testing and Materials, Soil Science Society of America, or U.S. Environmental Protection Agency [EPA]) are used, a PNNL cover page will not be provided unless there is a deviation from the established method.

Test instructions will be made available on the project SharePoint site.

Appendix B of this QAPjP lists additional analyses and measurements with their respective procedures, methods, and other relevant information.

Administrative quality assurance processes and procedures (e.g., chain-of-custody, custody logs, sample handling, storage and disposal, training) will be required from the onsite and offsite analytical laboratories and will be specified in the SOW.

#### 5.2.6 Well Drilling and Construction Procedures

S.M. Stoller will obtain well-drilling services through its procurement process. A SOW to S.M. Stoller specifies well drilling, characterization (aquifer and sediment sampling, etc.) and construction requirements. The well drilling, sediment samples collection, groundwater samples collection, water-level measurements, and notification to perform a geophysical logging/gyroscope well deviation survey (if required by the applicable test plan) is the responsibility of S.M. Stoller. These activities will be performed to S.M. Stoller procedures and/or to subcontractor procedures (e.g., conducting geophysical logging/gyroscope well deviation survey). S.M. Stoller Health and Safety, and QA procedures and waste management procedures will be followed during the drilling activity.

#### 5.2.7 Groundwater Sample Collection

Sampling during well drilling will be done by S.M. Stoller under the supervision of the Stoller field sampling organization or by Rifle IFC Site Project staff, Principal Investigators, or their designees. All other sampling conducted during field experiments will be done by Rifle IFC Site Project staff, Principal Investigators, or their designees. Quality requirements for sampling activities, including requirements for procedures, containers, transport, storage, chain-of-custody, and record requirements are specified in a Letter of Instruction to the S.M. Stoller field sampling organization.

Procedures are designed to reduce variability between sampling events and obtain representative samples, thereby maintaining consistent quality during groundwater sampling. The quality of the sampling operations is important to the ultimate quality of the data that the laboratory will obtain by following standard analytical procedures.

To assure that samples of known quality are obtained, controlled procedures based on standard methods for groundwater sampling will be used, whenever possible. The Rifle IFC Site Project Sampling and Analysis Technical Lead and project Quality Engineer will review and approve procedures before use for technical quality and consistency. In many cases, existing procedures can be used and incorporated in test plans by reference. Assessments will be performed by PNNL to further assure that procedures are followed to maintain sample quality and integrity (see Section 8.0).

#### 5.2.8 Water and Sediment Sample Collection Procedures

Groundwater sampling of a routine nature within this project will be done by Rifle IFC Site Project personnel. To assure that samples of known quality are obtained, Rifle IFC Site Project staff will be required to follow applicable Rifle IFC procedures based on standard methods for groundwater sampling whenever possible. PNNL will perform assessments to further assure that procedures are followed to maintain sample quality and integrity (see Section 8.0).

Sediment and water samples collected during drilling will be collected by or under the direction of Stoller Corporation, and in accordance with Stoller or subcontractor procedures. The quality requirements for sampling activities, including chain-of-custody, storage, and records requirements are specified in the SOW (or well data sheet). Scheduling sample container preparation, chain-of-custody and related paperwork will follow internal Rifle IFC Site Project procedures.

#### 5.2.9 Receiving and Handling Samples

Direction for sample receipt, handling, and storage at PNNL is provided in the SBMS subject area "Sample Handling, Archival, and Disposal" (PNNL 2007g).

Chain-of-custody for samples will be documented using a chain-of-custody form. An example of a chain-of-custody form is provided as an exhibit in CAWSRP. Chain of custody will be documented for moving samples from one facility to another, but not for moving samples within a facility or for samples analyzed at the field site or hand-carried from the field site to the Grand Junction Environmental Sciences Laboratory. Samples so handled will be documented in the onsite field LRB or data sheets.

Disposition of unused materials may include returning the material to the DOE Grand Junction facility or disposing of the material at the facility performing the sample analysis. Material returned to

the client will be documented by a chain-of-custody. Material disposed of at PNNL will be documented by standard waste paperwork (forms). See SBMS subject area, "<u>Waste, Managing</u>" (PNNL 2007i).

#### 5.2.10 Sediment Physical Analysis Procedures

Sediment physical analyses including moisture content, particle-size distribution, hydraulic conductivity, water retention, water content, bulk density, particle density, and matric potential will be performed as directed in the test plan by PNNL staff. Selected procedures are contained in the internal *Procedures for Ground-water Investigations* (PNL-MA-567) or on project-specific internal procedures for the Rifle IFC Site Project.

#### 5.2.11 Sediment Core Analysis Procedures

Sediment core analyses and column experiments will be performed by project participants as described in the test plan. Procedures are contained in the individual test plans, which will either provide a procedure or reference an existing procedure. Alternatively, for specialized analyses under development as part of scientific activities of the project, procedures may be documented as developed during sample analysis. Such procedures will be documented as described in Section 5.2.3 when work is completed.

#### 5.2.12 Geophysical Logging Procedures

Geophysical logging and gyroscope well-deviation surveys during well drilling will be performed by S.M. Stoller using its procedures, and as directed in the SOW as applicable. All other geophysical logging procedures will be performed by LBNL or other project participants according to documented test procedures.

## 6.0 Data Generation and Acquisition

## 6.1 Sampling Process Design (Experimental Design)

Experimental data generation and data-collection designs for each of the Rifle IFC Site Projects are described in individual work plans and sampling and analysis plans.

Routine sampling processes used to support the Rifle IFC Site Project studies will be in accordance with the waste management area sampling design, based on applicable regulatory requirements (e.g., UMTRCA, *Resource Conservation and Recovery Act* [RCRA] or CERCLA) and applying the DQO process in accordance with *Guidance on Systematic Planning Using the Data Quality Objectives Process* (*QA/G-4*) (EPA/240/B-06/001). Process descriptions will be included in sampling and analysis plans, along with the number of samples, when to sample, number of sample locations, number of quality control samples (field replicates, etc.), analysis methods and quality control criteria, and groundwater-level measurements.

#### 6.2 Sampling Methods

The procedures for collecting samples and identifying the sampling methods and equipment (including any implementation requirements), sample preservation requirements, decontamination procedures, and materials needed for projects involving physical sampling are described in the Rifle IFC Site Project study-specific work plans and procedures. Specific performance requirements for the methods are also described. If a failure in the sampling or measurement system occurs, documentation of and recovery from the failure will be documented in the project-specific LRB or controlled field book. The Rifle IFC Site Project study Principle Investigator is responsible for ensuring the corrective action is effective and documented.

Preparation and decontamination of sampling equipment, including the disposal of decontamination by-products; the selection and preparation of sample containers, sample volumes, and preservation methods; and maximum holding times to sample extraction and/or analysis is also Rifle IFC Site Project topic-specific and will be managed in accordance with EPA/SW-846 (as amended) or PNNL-specific procedures, as applicable. Waste generated as a result of the activities will be handled in accordance with SBMS subject area, "Waste, Managing" (PNNL 2007i).

Field sample collection, if applicable, will be done by PNNL, or Rifle IFC Site Project staff to specific procedures and test plans. PNNL will prepare, integrate, and coordinate sample collection schedules and constituent analysis of groundwater samples in accordance with monitoring plans and a specific procedure. The paperwork and instructions provided to the field personnel will include sample authorization forms, chain-of-custody forms, labels, and the groundwater sample reports. PNNL staff will track, oversee, and interface with the sampling organization to assure work is completed as specified.

#### 6.3 Sample Handling and Custody

Water samples will be collected by Rifle IFC Site Project staff in accordance with PNNL and/or approved Rifle IFC Site Project-specific procedures. Custody of field samples and receipt at the laboratory will be documented on the chain-of-custody forms in accordance with PNNL procedures. Also, shipping and transportation of the samples will be handled by PNNL in accordance with PNNL procedures and federal regulation.

## 7.0 Data Reduction, Verification, and Reporting

#### 7.1 Data Reduction

Data measured during technology project investigations are compiled, evaluated, and documented as described below. Samples and associated analyses will be scheduled and tracked to assure successful sample collection. Selected data may be loaded into the Rifle IFC Project database, as identified in the respective test plan.

Verification of analytical data is performed in accordance with Appendix A of this QAPjP, as appropriate. Results are reviewed to assure the reliability and validity of the field and laboratory measurements based on accuracy, precision, and detection limits. Representativeness, completeness, and

comparability may also be evaluated for overall quality. These parameters are evaluated through laboratory quality control checks, replicate sampling and analyses, analysis of blind standards and blanks, and/or interlaboratory comparison. Acceptance criteria are established for each of these parameters in Appendix A of this QAPjP, the *Environmental Sciences Laboratory QA Plan* (QAP ESL, current revision), and/or in specific test plans. When a parameter is outside the criteria, corrective actions are taken to prevent a future occurrence and any data impacted is appropriately flagged.

When the data review identifies suspect data, those data are investigated to establish whether they reflect true conditions or an error. If appropriate and as determined by the Project Manager or delegate, a remedial design report is initiated in accordance with procedure DA-3, *Data Review Procedure* (see PNL-MA-567) or another appropriate project-specific method.

## 7.2 Sample Data Tracking and Verification

The process for tracking and scheduling sampling and analysis requirements, sampling field activities, chains of custody, and laboratory analysis is managed using a variety of electronic data management tools. Data are received from the analytical laboratories in electronic and/or hard copy form.

A central, web-accessible SharePoint site or database for all samples, characterization measurements, and experimental data, which enables remote-collaborative efforts will be used. Raw data, sampling metadata, and instrument calibrations will be stored to allow an auditable, reproducible link between field measurements and finalized data. Clear linkage between field data and numerical predictive models will be established to allow reproducibility. Selected wells and sensors will be linked to an automated data acquisition infrastructure that will utilize a cell-phone wireless network feeding the System Operation and Analysis at Remote Sites (SOARS) real-time data collection system. A separate Internet-based network will support an electronic notebook and logging of key field events and activities by site personnel. Key sample data tracking and verification elements of this approach include the following:

- *A centrally managed data repository.* This will consist of an organized set of spreadsheets or a number of relational databases that will house all data (geochemical, hydrological, geophysical, microbiological, environmental and experimental) collected as part of the Rifle IFC Site Project. These spreadsheets or databases will contain information on sensors, analytical procedures and instruments consisting of the raw data and calibration equations used.
- *Inventories of solid and liquid samples*. The availability of solid and liquid sample data, their analytical characteristics, and other research results generated on them will be readily traceable and linked through the SharePoint site, spreadsheets, web interface or, associated databases.
- Integration of additional data sources. Ongoing regulatory driven data acquisition at the Rifle, Colorado, processing site has resulted in a considerable amount of data (e.g., Geospatial Environmental Mapping System [GEMS]
  <u>http://gems.lm.doe.gov/imf/imf.jsp?site=gems\_continental\_us</u>) which will be used in the overall analyses of experiments performed by the Rifle IFC Site Project. These data are contained in other databases that will be accessed via links from the IFC data management system. In addition, a number of parallel field efforts will generate useful data that will be integrated into the IFC database as appropriate.
### 7.3 Sample Data and Tracking for Sediment and Other Media Samples

Completed data packages for sediment and other media samples will be verified by PNNL personnel after project participants provide data to PNNL to upload to the SharePoint site. Verification will consist of verifying required deliverables for completeness, required quality control results, and the availability of other documentation such as chain-of-custody forms, and case narratives that describe any issues related to the sample analyses. Verification may also include evaluating and qualifying results based on holding times, method blanks, matrix spikes, laboratory control samples, laboratory duplicates, and chemical and tracer recoveries, as appropriate to the methods used. No other verification/validation or calculation checks will be performed. At least 10% of all data types (i.e., volatile organic chemicals, semi-volatile organic chemicals, metal, etc.) will be verified. Verification will be documented on checklists to be included in the project files.

### 7.4 Data Reporting

Data measured during the project are compiled, evaluated, and documented as described below. When the data review identifies suspect data, those data are investigated to establish whether they reflect true conditions or an error.

All data reported shall be traceable to the M&TE and procedure (including procedure revisions) or test plan used, and if the reported results are quantitative, a valid calibration as appropriate. The analyst shall sign or initial and date the data reports unless the results printed by the instrument include identification of the analyst and date, or unless the data are linked to or include metadata with this same information. A staff member other than the person who performed the work, and is knowledgeable in the area being reviewed, shall review the data before results are reported.

Interpretative data, test results, and reports will be released through the information release process in accordance with the SBMS subject area, "<u>Publishing Scientific and Technical Information</u>" (PNNL 2007d) or in accordance with accepted analogous protocols at participating institutions.

## 8.0 Analytical Quality Control Checks

Analytical quality control checks are performed on internal and external samples. A summary of quality control check samples is outlined in Appendix A of this QAPjP, the *Environmental Sciences Laboratory QA Plan* (QAP ESL, current revision), and/or in specific test plans. Internal quality control data are generated when the analytical laboratory prepares quality control samples to monitor the quality of its analyses.

Quality control activities needed for sampling, laboratory (internal and external) and field analysis, or measurement technique will be defined in the appropriate Rifle IFC Site Project test plans. For each required quality control activity, the associated method, acceptance criteria, and corrective action will be listed. Also, for the field and laboratory quality control activities included, but not limited too, are the use of blanks, duplicates, matrix spikes, laboratory control samples, and surrogates in the plans. The experiment-specific QA plans also identify the procedure, formulae, or references for calculating the percent recovery (if applicable), bias, and precision.

## 9.0 Assessments

Assessments are performed to gather results that can be evaluated to measure the effectiveness of the quality systems and processes implemented by the project. Assessments will be performed periodically during the year. The following types of assessments may be used at varying frequencies during the year:

- Management self-assessment an assessment performed by those immediately responsible for overseeing and/or performing the work to establish whether policies, practices, and procedures are adequate for assuring results needed.
- Management independent assessment an assessment performed by an individual or group independent of the work performed to assure that policies, practices, and procedures are adequate for assuring results needed.
- Technical independent assessment an assessment performed by an individual or group technically competent to do the work but independent of the work being performed to assure qualitative and quantitative aspects of the work are accomplished according to documented specifications. Technical independent assessments are conducted by Field Research Executive Committee (FREC). (Appendix D provides the management plan for IFCs implemented by DOE SC.)

Data quality assessments are conducted as project quality control checks. The focus of data quality assessments is independent verification of reported results. Data quality is routinely evaluated through technical review, including review of documents submitted for publication. If the complexity and/or significance of the work performed warrants it, the Project Manager will direct the QA representative and/or another staff member to conduct an additional quality assessment. The assessment is documented and retained in the project records. Documentation of the above assessments, as well as any external assessments performed, is maintained as project records. The Project Manager is responsible for ensuring that any deficiencies are corrected in a timely manner.

## 9.1 Assessment Planning and Documentation

The project management team (including Project Manager, Technical Leads, and appropriate project staff) plans assessments in consultation with the project Quality Engineer. An assessment schedule will be developed by the project Quality Engineer with Project Manager approval. Assessments may be performed by the project staff, project management, and/or the Quality Engineer in accordance with the SBMS subject area, "Planning, Assessment, and Analysis, Section 2: Performance Assessment" (PNNL 2007b). The assessor plans the assessment on a Self-Assessment Planning Form (see Figure 9.1 for an example) where the scope of the assessment, topic, and supporting references are documented in the plan. A unique identification number is assigned by the PNNL Assessment Tracking System (ATS) to the plan and entered on an assessment log sheet. The Project Manager (or delegate) then approves the plan. Results of assessments will be documented on a Self-Assessment Results Form (see Figure 9.2 for an example).

#### SELF-ASSESSMENT PLANNING FORM

| Scope & Location: (General: Maintenance, Operations,    | I.D. Number: (ATS Number or other Unique Tracking      |
|---|--|
|   | Number)  |
| <b>Topic:</b> ( <i>Describe what will be assessed</i> ) | <b>Date:</b> ( <i>Date planning form is prepared</i> ) |

**References:** (*Cite Source Documents for Performance Expectations i.e.*, Regulation, Environmental Permit, DOE Order, A-Manual, Standards Based Management System [SBMS], Requirements, Procedures and Guidelines [RPG]).

#### **Performance Expectations**

Criteria developed from Source Documents that will be applied throughout the assessment. Each criteria/expectation will have the reference enclosed in parenthesis at the end of the criteria/expectation statement (e.g., DOE Order 5480.19, SBMS, RPG). Performance expectations should be limited to six maximum to allow the assessment to remain focused. Additional Planning Forms can be completed to expand the scope of a particular assessment.

| 1. |  |
|----|--|
| 2. |  |
| 3. |  |
| 4. |  |
| 5. |  |
| 6. |  |

Procedure: (*Perform the following as applicable for the assessment*) Review assessment planning form

• Review applicable procedure/requirements. (references)

- Conduct performance tests and data validation.
- Observe the activity controlled by the procedure.
- Interview appropriate personnel about requirements and practices.
- Record observations based on comparison to plan.
- Document the results after receiving final information on the Self-Assessment Results form.

| <b>Basics for the</b> | [] Planned    | [] | Lessons Learned |
|-----------------------|---------------|----|-----------------|
| Assessment:           | [] Responsive | [] | Other           |

Work Package Number (optional):

Assessment Requestor/Authorizing Person:

Assessor(s):

Figure 9.1. Self-Assessment Planning Form

### SELF-ASSESSMENT RESULTS

| Assessor:            | I.D. Number:                                      |
|----------------------|---|
| Assessment Location: | <b>Date:</b> ( <i>Date assessment performed</i> ) |

Results

(Related to Associated Performance Expectations)

#### **Subsequent Actions** (*Related to Associated Results*)

| Assigned Action   | Action Owner                        | Due Date          |
|---|-------------------------------------|-------------------|
| 1.  |                                     |                   |
| 2.  |                                     |                   |
| 3.  |                                     |                   |
| 4.  |                                     |                   |
| Actions Assigned By:  |                                     | Date:             |
| <b>Completion</b> ( <i>To be signed by Lead Assessor when assessme</i><br><b>Signature:</b><br><b>Date:</b> | ent is completed.)                  |                   |
| <b>Completion</b> ( <i>To be signed by Manager when assessment is</i>                                       | completed and all actions have been | entered into ATS) |
| Signature:<br>Date:   |                                     |                   |

Figure 9.2. Self-Assessment Results

The corrective action and action owner will be documented in the assessment report. The action owners will be assigned by the Project Manager (or delegate). An action item log will be maintained by the project Quality Engineer to track and close out actions. The Project Manager will prioritize the corrective actions, which will then be verified by the project Quality Engineer. When the corrective actions have been closed, the Project Manager will sign the assessment report. The assessment plan and report will be distributed to the appropriate staff, Project Manager, and project records.

## 9.2 Subcontractor/Collaborator Assessments

If PNNL requests work via subcontractors, periodic assessments of these subcontractors are performed as an oversight function or prior to contract award in accordance with the internal acquisition quality procedures. Provisions are made in the SOW for oversight assessment activities to be performed as necessary.

The results of all subcontractor assessments (including surveillances and audits) will be made available to project and line management, individuals contacted, and the client as requested. The corrective action tracking, corrective action and closure response will be in accordance with the internal acquisition quality procedures. The official assessment report files and responses (audits and surveillances) are maintained in the PNNL Suppliers history file by the Quality Assurance Services group.

Periodic assessments of well drilling and construction, drilling and sampling-related activities, and the Environmental Sciences Laboratory may also be performed in accordance with the requirements discussed above.

## **10.0** Preventive Equipment Maintenance

Subcontracted organizations and collaborators will be required to implement preventive maintenance on their equipment to mitigate the possibility of down-time affecting cost and schedule. This will be specified in the SOW to the respective organizations.

## 11.0 Specific Routine Procedures Used to Assess Data Precision, Accuracy, and Completeness

The evaluation of laboratory precision, accuracy, and completeness is accomplished during the verification process performed upon receipt of data (see Section 7.0 of this plan).

## **12.0** Corrective Action

### 12.1 Project Corrective Actions Resulting from Assessments

As part of the continuous improvement processes initiated by the project management team, assessments will be tracked and improvement actions identified and prioritized. The <u>Assessment Tracking</u> <u>System (ATS)</u> is the process used by this master project for tracking and managing assessments, including determining conditions and the development of actions. ATS supports the identification, control, and correction of items, services, and processes that do not meet established requirements. The SBMS subject area, "<u>Assessment Management</u>" (PNNL 2005a) documents this corrective action management process for handling and documenting events and assessments, including those that must be tracked in ATS (such as formal project reviews or audits performed by the client or their representative; or management-initiated assessments, etc.). If immediate corrective action is required, the quality problem will be entered directly into the ATS and corrective actions taken as specified in Section 12.2.

#### **12.2 Unplanned Deviations**

Corrective action must be initiated by the Project Manager or cognizant Task Leader when <u>unplanned</u> deviations from procedural, contractual, regulatory requirements or construction specifications occur. These deviations will be documented by documenting the quality problem information directly into the ATS in accordance with the SBMS subject area, "<u>Quality Problem Reporting</u>" (PNNL 2005c). The assessment must describe the problem, the cause of the deviation, the impact of the problem, and corrective action needed to remedy the immediate problem and to prevent recurrence.

Subcontractors and collaborators will be required to have a system in place to identify, correct, and prevent recurrence of contractual, procedural or regulatory requirement(s) deviations, and to notify the PNNL point-of-contact specified when such an event occurs. These requirements will be passed on in a SOW to the subcontractors.

#### **12.3** Planned Deviations

Planned deviations from procedures that are documented (including justification) and approved by the Project Manager or Task Leader <u>in advance</u> do not constitute a deficiency and do not require generation of an assessment item. Documentation may consist of a hard copy e-mail or memo to the Project Manager or Task Leader. This documentation must include either an approval signature if on a memo or electronic approval via a reply to the e-mail indicating such approval. Development of procedures or measurements in process (as described above) also does not constitute a deficiency and do not require generation of an assessment item.

#### **12.4** Measuring and Test Equipment Calibration Discrepancies

Subcontractors will be required to maintain a system for identifying calibration discrepancies and tracing data or samples that may have been affected. Subcontractors will be required, via a SOW, to notify the PNNL point-of-contact as soon as possible when such an incident occurs. PNNL will perform periodic assessments to assess the effectiveness of subcontractor procedures and processes for calibration control.

Rifle IFC Site Project staff must investigate instruments or equipment found to be operating outside acceptable operating ranges (as specified in the applicable technical procedure or manufacturer's instructions) and issues must be addressed in accordance with the SBMS subject area, "Quality Problem Reporting" (PNNL 2005c). If as-found data on an instrument's calibration report are determined to be out of tolerance during the review and acceptance process, and the contract-supplier documents were submitted in response to quality requirements, an "Out-of-Tolerance Notification" will be generated using the ATS in accordance with the SBMS subject area, "<u>Assessment Management</u>" (PNNL 2005a). Project staff must then determine if there was any impact on data. When it is determined from the calibration verification process that Category 1 or 2 M&TE is out of tolerance, project staff should proceed with the evaluation to determine impact on data and document the results with appropriate justification.

## 13.0 Quality Assurance Reports to Management

Quality-related problems identified by project personnel must be immediately reported to project management for resolution. Any problems involving data quality, sample integrity, or test measurements will be thoroughly documented by a remedial design report and/or a problem and discrepancies form and communicated to the appropriate Task Leader and Project Manager for resolution.

Quality activities, such as project improvement efforts; significant deficiencies identified and associated corrective actions; and assessment result summaries will be reported to the Project Manager. When major quality problems are identified, they shall be reported to the Project Manager. Surveillance plans and surveillance results are provided to the Project Manager and Task Manager after a surveillance event.

Significant quality-related problems that may affect customer satisfaction shall be communicated to the Product Line Manager by the Project Manager.

## 14.0 Records

### 14.1 Records Control

SBMS definitions of project records and record material apply to this project. As stated in the SBMS subject area, "<u>Records Management</u>" (PNNL 2005d), project records are any recorded information relating to a specific research project. Record material includes information, regardless of its media (e.g., hard copy, electronic, microfilm), that is created or received in connection with Pacific Northwest Division business or research activities and is preserved for its value. Record material includes documentation of research and administrative functions, policies, decisions, procedures, operations, or other activities.

**Note**: E-mail that is record material must be printed out and maintained as the record copy unless the e-mail is saved directly into the PNNL <u>Total Records Information Management (TRIM)</u> System. Record material that is not stored in field notebooks or laboratory records books (see Section 19.5 of this QAPjP) or is not electronic data gathered from sensors or instruments in the field and/or a laboratory (see Section 14.3 of this QAPjP) such as project-specific field data forms, shall be scanned and managed as PDF files in accordance with Section 14.3. The record material shall be scanned and archived at least quarterly per year or more often, such as weekly or monthly, if the accumulation of material is significant and inadvertent damage or loss would cause irreparable damage to the project.

Records that document sampling subcontractor activities, analytical results, verification and compliance checks, quarterly and annual reports, test plans and associated results, groundwater monitoring plans, and assessment reports will be maintained as project records. Individual monitoring plans and work plans may identify other records requirements. Project records will be legible, identifiable, and maintained in accordance with the SBMS subject area, "<u>Records Management</u>" (PNNL 2005d). Test results documented in LRBs will be reviewed semi-annually by a technically qualified individual who did not perform the work. The reviewer will verify there is sufficient detail to retrace the investigation and confirm the results.

The Project Records Specialist prepares and submits a Records Inventory and Disposition Schedule file index for review and approval by the records management representative and Quality Engineer. The records custodian reviews and updates the Records Inventory and Disposition Schedule annually at a minimum, or when a major change to the program occurs. Records retention schedules shall be based on requirements of the *Hanford Federal Facility Agreement and Consent Order* (Tri-Party Agreement) (Ecology et al. 1989), which requires the retention of records for 10 years after termination of the Tri-Party Agreement.

#### 14.2 **Records Transfer to Storage**

On an annual basis, the records custodian will transfer to storage inactive records as identified by the Technical Lead that are not required for day-to-day operations. Sampling and analysis plans, assessments, and special project correspondences will be maintained by project staff until the activity or project is complete. The Project Records Specialist generates the internal form (e.g., Records Transfer/ Data Input [RTDI] Form). The records management representative will sign the RTDI form as acknowledging receipt of the records and return a copy of this form to the records custodian. The RTDI form is then placed in project records.

Within 90 days of project completion or termination, records shall be transferred to storage and/or the client. The Project Records Specialist completes the appropriate internal form (e.g., RTDI form). The records management representative will sign the RTDI form as acknowledgment of the receipt of the records and return a copy of the form to the records custodian. The RTDI form is then placed in project records.

#### 14.3 Electronic Data/Records Management

Electronic data gathered from sensors or instruments in the field and/or a laboratory will be maintained and managed appropriately to allow for reproducible results. Electronic data that are directly delivered and/or used in analysis, or are delivered to the customer, will be maintained as project records in accordance with the requirements of the SBMS subject area, "<u>Records Management</u>" (PNNL 2005c). Electronic data produced by instrumentation or sensors are usually stored on that instrument and are only

usable by the system itself. It is necessary for the electronic data to be transferred, without error, to a form that can be used by a variety of software applications. An example would be to transfer an ASCII (American Standard Code for Information Exchange) file into a Microsoft Excel<sup>®</sup> file<sup>7</sup>. To ensure the data transfer process has occurred in an acceptable manner, a review of a representative sample with sufficient data points to provide confidence that the data have been transferred properly shall occur. The review method used and results obtained shall be documented and retained as project records in the LRB, in accordance with Section 19.5 of this plan. For data retrieval, the staff member shall record the use of the data on the media used to store the raw data and in the project records. The staff member shall ensure that unauthorized modifications are not made to the data during its use. The method of control shall be documented in the project records by the staff member. The staff member shall ensure that a backup of the data is maintained in the project records. Use of the data in software applications shall be documented, along with the software application name and version number.

Electronic data shall be archived and saved as project records based on the project's record-retention period. When the project records are required to be maintained for a minimum of 10 years, after the close of the project, saving the raw electronic data files to a CD/DVD is sufficient. When the project's record retention requirements are longer then 10 years, the raw data files should be saved either to magnetic media (TRIM, tape) or optical media (CD, DVD). The <u>TRIM</u> system is one option for storing raw data files and is approved for projects that have a permanent-retention period.

Backup and archive processes shall be followed for maintaining the data during the life of the project. Electronic data backups shall be performed nightly, in accordance with the requirements identified by the PNNL IT Computing Services - <u>InfoSource</u> website. The computer-backup procedures on the PNNL InfoSource website for <u>Data Backup Options</u> shall be followed based on the type of computer or server on which the data are stored. The data backup process is identified in the following sections.

#### 14.3.1 Workstations

PNNL staff are responsible for ensuring the data on the computers they use are regularly backed up. There are three options for backing up these data:

- 1. The staff member can sign up for one of the PNNL <u>workstation backup and restore (WBR)</u> services: <u>Connected DataProtector</u> for Windows, <u>WBR Mac</u> for Macintosh, or <u>WBR Networker</u> for all other systems. WBR is free to each staff member for one workstation. Additional backup subscriptions are available for a small monthly fee. (See the WBR website at http://infosource.pnl.gov/Network/services/wbr/default.stm for restore instructions.) The maximum backup size is 100 GB for Windows workstations.
- 2. A <u>network shared folder</u> may be used to store files on a PNNL network file server. Network shared folders are backed up nightly. To retrieve files from a backup, request a file restore by calling the PNNL Help Desk at 375-6789 or sending them an e-mail. The Help Desk technicians will need the complete name of the shared folder (for example, \\pnl10\projects) and the name and date of the file or directory that needs to be restored.

<sup>&</sup>lt;sup>7</sup> Excel is a registered trademark of Microsoft Corporation.

3. Staff may manually copy files to floppy disks, CDs, or DVDs. Most computers purchased through the Managed Hardware Program come with large-capacity floppy drives, CD-RW drives, and/or DVD drives. A CD can store 600 MB or more; DVDs 4.7 GB. Either of these methods is suitable for backing up important data files, but not recommended for backing up the entire system.

#### 14.3.2 Servers

The data backup options for servers include the following:

- 1. The <u>WBR</u> service. For a small monthly fee, WBR performs a full backup of all the project's programs and data. (See the WBR website for restore instructions.)
- 2. Backing up to Zip disks or to a tape drive connected to the server. If a tape drive connected to the project server is used, refer to the manufacturer's instructions for setting up backup schedules and performing restores.

Data archiving shall occur at least every 2 weeks; it is recommended archiving occur at least once a week. The electronic data shall be archived to a CD/DVD and kept in the project working files until the electronic data are no longer being used; at that point, the electronic data shall be moved to TRIM when longer-storage retention is required by the records requirements.

## **15.0** Procurement Control

Quality-affecting materials (e.g., calibration standards, chemicals) or services (e.g., calibration, analytical services, or other subcontracts for technical services) will be obtained in accordance with SBMS subject area, "<u>Purchasing Goods and Services</u>" (PNNL 2007e). For this project, the majority of procurements will result in purchases of services such as drilling, sampling, and analytical services. All procurements will be obtained in accordance with SBMS subject area, "<u>Purchasing Goods and Services</u>" (PNNL 2007e). SOWs for purchasing services shall be reviewed and signed by the project Quality Engineer to assure consistency of QA requirements specified to subcontractors with project quality standards in this plan.

### 15.1 Groundwater Sampling

Test plan procedures shall be used within the project or by collaborators to obtain sample collection and water-level measurements. The test plan will include requirements for sample collection, sample handling, sample labeling, custody of the samples in the field to delivery to the analytical laboratory or shipper, and water-level measurements. The test plan procedure will pass on the requirements of the *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA/240/B-01/003) and HASQARD (DOE-RL 1998). A review must be performed by the Quality Engineer during the planning stages and preparation of the test plan procedure.

### 15.2 Groundwater and/or Sediment Analytical Measurements

If the groundwater or sediment analysis will be conducted by personnel not involved in the development of the test plan procedures, work package authorizations, work orders (WOs), or purchase orders (POs), as applicable, shall be used to obtain the analytical services. A letter of instruction (LOI) or SOW must accompany each WO, WP, or PO. A review must be performed by the Quality Engineer during the planning stages and preparation of the SOW/LOI. The work authorization document must define the data quality and any additional project requirements associated with the service requested. The data quality requirements should include a description of the quality control samples for each analysis for determining the level of possible contamination from preparation and analysis. The project requirements should include information on analysis method, calibration standards traceable to the National Standards and Technology or other recognized source of standards appropriate to the analyses being performed, sample turnaround time and reporting requirements, and disposal requirements for remaining sample material and the waste from the process. The LOI/SOW will include the minimum requirements of the *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA/240/B-01/003) and HASQARD (DOE-RL 1998) to the analyst and/or requirements of this plan as appropriate.

## 15.3 Other Hanford Site Contractor Services

While it is unlikely the Rifle IFC Site Project will use other Hanford Site contractor services, this section will be followed if those services are needed. An electronic requisition will be generated by project staff accompanied by a work authorization document (LOI or SOW). The work authorization document will describe the requirements for the requested services. The SOW will pass on the requirements of the *EPA Requirements for Quality Assurance Project Plans (QA/R-5)* (EPA/240/B-01/003) and HASQARD (DOE-RL 1998) to the subcontractor. A review must be performed by the Quality Engineer during the planning stages and preparation of the LOI or SOW.

## 16.0 Staff Training

Staff performing activities affecting quality shall be issued documented training assignments, including applicable project administrative and technical procedures and this plan.

- 1. The Project Manager and staff members will assess project-specific training needs. The assessment will include evaluating cumulative staff training records.
- 2. The Project Manager will assign reading and/or briefings of procedures as needed. If training is assessed and the need for formalized training is identified, the staff member will be scheduled to attend a formal training class.
- 3. Training will be documented on either a briefing document; an individual on-the-job training (OJT) form; a reading assignment documentation form; or a group OJT or reading assignment documentation form. These forms are available internally to PNNL staff. Documentation shall be sent to the PNNL Laboratory Training Coordinator for input into the training database. The training database will contain the record copy of project staff training.

The Rifle IFC Site Project shall utilize personnel who are knowledgeable and possess adequate technical, managerial or professional skills to perform all their assigned tasks. The Project Manager will identify any additional specific project-related processes that will require the project staff training and qualification, and who will be responsible for assuring the project-specific training will be developed, delivered, and changes managed in accordance with the SBMS subject area, "Training Design, Development, Implementation and Evaluation" (PNNL 2002). The project shall maintain training documentation for project-required coursework or OJT taken by staff that is not capable of being tracked in PNNL's training database in accordance with the SBMS subject area, "Training and Qualification for Staff and Non-Staff" (PNNL 2005e).

The Project Manager, or assigned delegate, shall inform the immediate manager of project staff of his/her requirement to take project-required training and assure that the training has been completed prior to project staff conducting work that requires the training. The immediate manager of project staff, or assigned delegate, shall record the need for identified project-required training, and assuring training (and retraining for changes) records (for both Laboratory-level and project-specific training) will be maintained in accordance with the SBMS subject area, "Training and Qualification for Staff and Non-Staff" (PNNL 2005e).

The development of software products that require complex or unfamiliar interactions with users and operators should include a comprehensive plan for training. The training plan should include the following:

- a) A description of the populations to be trained, the training objectives for each population, and the content to be covered in the training.
- b) An estimate of the amount of resources necessary for training development, delivery, and time expenditures.
- c) Procedures for evaluating the effectiveness of the training and for making training modifications.

The Project Manager has identified the following project-specific training requirements on which project core team members will have been briefed:

- The Project Management Plan
- The QAPjP
- Field Site Management Plan
- Health and Safety Plan
- Communications and Community Interaction Plan.

The project shall maintain training documentation for project-required coursework, or OJT taken by staff, which is not capable of being tracked in the Laboratory's training database in accordance with the SBMS subject area, "Training and Qualification for Staff and Non-Staff" (PNNL 2005e).

## **17.0 Software Control**

For the purpose of design activities covered by the activities identified in this plan, software is defined as computer programs—including computer programs embedded in firmware (see the SBMS

subject area, "<u>Software</u>" [PNNL 2007h]). Excluded is software that is an integral part of firmware or equipment, where all software maintenance is performed by the vendor and the software is verified as an integral part of the system (e.g., calibration with known standard materials). The software clause (<u>QA-197b</u>) will be included in any SOWs, at a minimum, and possibly with additional clarification, when requested by the vendor.

All software applications used for the projects covered under this plan will be reviewed and identified as non-safety software. The grading process for software will be recorded and copies for each application will be maintained as project records for each project that falls under this plan. Software applications that will follow this plan do not have the potential to be identified as Safety Software and will not be identified as such and do not need to follow the SBMS subject area, "Safety Software" (PNNL 2007f) requirements.

### 17.1 Software and Software Applications

Software applications identified for the project in this plan will perform the work activities identified in the following sections that pertain to custom developed, configurable, and acquired/legacy software.

#### 17.1.1 Minimum Documentation Requirements

To ensure implementation of the software satisfies requirements, the following documentation is required as a minimum for all software applications. The rigor of the documentation will be decided by project management based on a graded approach of the software application.

The grading of the requirements will be based on the risk associated with the failure of the intended use of the software. There are three (3) categories identified with the grading of the software requirements are: Detailed, Functional or Summary level. The grading and category level of each application under this plan will be identified in the appropriate documentation.

- a. Software Requirements Specifications (SRS)
- b. Software Design Description (SDD)
- c. Verification and Validation Plan (VVP)
- d. Verification and Validation Report (VVR)
- e. Configuration Management Plan
  - 1. A problem reporting and corrective action tracking system will be identified with the CMP documentation.
  - 2. Data management process will also be identified, when applicable
- f. Procurement Contractual documentation, when applicable.

#### 17.1.2 Software Requirements Specification

The Software Requirements Specification (SRS) shall clearly and precisely describe each of the essential requirements (functions, performances, design constraints, and attributes) of the software and the external interfaces. Each requirement shall be defined such that its achievement is capable of being objectively verified and validated by a prescribed method (e.g., inspection, analysis, demonstration, or

test). The SRS will be developed with less rigor when the software being used is configurable, acquired but slightly customizable, or legacy software.

The SRS is subject to the Software Requirements Review (SRR) when needed and will be documented. The SRS is subject to a Software Requirements Review by the client when the software is the deliverable and not just used to provide analysis or results for a clients deliverable. The client acceptance of the requirements will be documented, when required.

#### 17.1.3 Software Design Description

The Software Design Document (SDD) shall depict how the software will be structured to satisfy the requirements in the SRS. The SDD shall describe the components and subcomponents of the software design, including databases and internal interfaces. The SDD is a technical description of how the software will meet the requirements established in the SRS. The most important function of the SDD is to describe a decomposition of the whole system into components (subsystems, segments, etc.). In addition, it should document the rationale for the more important design decisions to facilitate understanding of the system structure.

The SDD will describe major system features such as databases, diagnostics, external and internal interfaces, as well as the overall structure of the design. It involves descriptions of the operating environment, timing, system throughput, tables, sizing, centralized or distributed processing, extent of parallelism, client/server, reusable objects library, program design language, prototypes, modeling, and simulation, etc. The SDD will also describe any input and output data that may be required.

The SDD will be baselined after each significant review. A new version containing a more detailed design description is developed for each subsequent review when new enhancements or defect fixes are incorporated.

The SDD will be developed with less rigor when the software being used is configurable, acquired but slightly customizable, or legacy software. The SDD is used to help design new enhancements or defect fixes when the design involves custom-developed code. Flow charts and/or flow diagrams can aid in the development and documentation of the design and when custom development is minimal can be used as the software design.

The SDD is subject to the Software Design Review, when needed and will be documented.

#### 17.1.4 Verification and Validation Plan

The Verification and Validation Plan (VVP) shall identify and describe the methods (e.g., inspection, analysis, demonstration, or tests) to be used:

- 1. To verify the following:
  - Requirements in the SRS have been approved by an appropriate authority
  - Requirements in the SRS are implemented in the design expressed in the SDD
  - Design(s) expressed in the SDD is implemented in the code.
- 2. To validate that the code, when executed, complies with the requirements expressed in the SRS.

The VVP describes the overall plan for the verification and validation of the software/modeling and will be produced and reviewed incrementally for software applications. The tasks, methods, and criteria for verification and validation will be described in the appropriate VVPs for each software application.

The VVP will be used to document the testing standards and practices as they are defined in each application VVP. The VVP will explain the scope of the validation testing to ensure the baseline requirements are met; and explain the stages of development that will require customer review, and the extent of the verification that will precede such a review.

The VVP will specify minimum test documentation requirements for each test performed. Additionally, a section of the VVP will identify a verification matrix where the requirements are listed with their corresponding test identified in the VVP. A matrix will be maintained during the life of the software and will be used to verify all the requirements have been met, identified, and tested.

The contents of the VVP will be evaluated at the Verification and Validation Plan Review (V&VPR) prior to testing. A V&VPR will be conducted when significant changes are made to the project baseline. The V&VPR will be used to identify all changes to be tested and to pass on pertinent information to the appropriate testing staff.

#### 17.1.5 Verification and Validation Report

The VVR summarizes the observed status of the software as a result of the execution of the VVP. The VVR should include the following information:

- 1. Summary of all life- cycle V&V tasks.
- 2. Summary of task results.
- 3. Summary of anomalies and resolutions.
- 4. Assessment of overall software quality.
- 5. Summary from the verification matrix.
- 6. Recommendations such as whether the software is, or is not, ready for operational use.

The report may be a full report or a summary (depending upon the grading of the software).

#### 17.1.6 User Documentation

User documentation will be developed for applications where the code is part of the deliverable.

#### 17.1.7 Configuration Management Plan

The Configuration Management Plan (CMP) shall document methods to be used for identifying software items, controlling and implementing changes, and recording and reporting change implementation status. The CMP should describe the tasks, methodology, and tools required to assure that adequate configuration management procedures and controls are documented and are being implemented correctly. If the CMP is not a stand-alone document, and is included in the Quality Assurance Plan or Project Management Plan (PMP), it is not necessary that the QA organizational element prepare the CMP; however, it is essential that one exist for each project or set of applications

under each project. The process of data management should also be identified in the CMP, when data input is used to produce results and the application is not the deliverable.

The CMP should describe the methods to be used for the following:

- Identifying all the configuration items (software modules, documents, data, etc).
- Controlling and implementing changes.
- Recording and reporting change and problem reports implementation status.
- Conducting configuration audits when appropriate.
- Identifying review and approval cycles, as well as signature authority.
- Identifying the personnel responsible for maintaining the baselines and distributing the CMP.

The CMP shall contain the information identified in the SBMS subject area, "<u>Software</u>" (PNNL 2007h) for "<u>Software Maintenance</u>." A summary of the requirements for maintaining software are as follows:

- Track defects and requests for changes
- Plan and approve software updates and changes
- Modify software and test
- Maintain source code and documentation.

#### 17.1.8 Other Documentation

Other specific project plans for each project under this plan may include the following:

- PMP
- QAPjP
- Security Plan.

<u>PMP</u>. The PMP can be used as the highest-level planning document governing a project, or could be subordinate within a larger set of plans. The PMP should identify all technical and managerial activities associated with the project. The PMP should specify the items, which should be reviewed and assessed by the Quality Engineer. The PMP should identify the risks associated with the use of the software if a failure was to occur, and the steps to mitigate the identified risks.

<u>Security Plan</u>. A Security Plan is only required if any of the software tools are going to be accessible on the internal PNNL sites.

<u>Risk Identification and Mitigation</u>. Specific risk and hazards that pertain to the maintenance, development, and/or use of software will be identified and documented with the project records associated with the task that required the software. The plans describe how to manage and mitigate the risks, and document the hazards. An example of a possible risk and management of that risk is identified below.

<u>RISK EXAMPLE</u>: The primary risk posed by use of this software is that a mistake in the software design or implementation could result in the calculation of an erroneous result, resulting in one or more of the following undesirable outcomes:

- For projects in progress, adverse impacts to project budget and schedule as corrections are made and calculations repeated to correct the mistake.
- For completed projects, invalid regulatory products that rely on the calculations performed with the software.
- Damage to the reputation of the Laboratory.

<u>RISK MANGAGEMENT EXAMPLE</u>: The primary means to minimize the risk of software errors of consequence are as follows:

- Adherence to the processes defined in this QAPjP
- Development and execution of a software test plan
- Timely identification, response, and communication to affected parties regarding software errors and anomalies discovered by PNNL staff involved in use, maintenance, and software development.

## 17.2 Software Use in Analysis

This section applies to use of software of any kind by this project to conduct analyses delivered, or in support of a deliverable to the customer. Included in this definition are data analysis tools including spreadsheets and statistical analysis software, databases, modeling and simulation tools. Excluded are software productivity tools such as word processors and spreadsheets when no automated calculations, macros, or scripts are used. The activities under this plan shall conduct work in accord with requirements for the control of software used in analyses as defined in the SBMS subject area, "<u>Software</u>" (PNNL 2007h) based on the risk associated with the use of the software. Using software to conduct analysis requires the following:

- Risks are identified
- Reviewers are identified to review the results and implementation of the software
- Analysis is planned
- Basis for the validation/review is documented
- Analysis is conducted
- Results are validated by the identified independent reviewer and review results are documented.

## **17.3 Utility Calculations**

The purpose of this section is to define a uniform method for documenting the quality controls in place when using software packages (e.g., Excel<sup>®</sup>, Mathematica<sup>®8</sup>, Matlab<sup>®</sup>, Mathcad<sup>®</sup>, etc. known as Utility Calculations) for calculations that are a significant part of a client deliverable, but not classified as

<sup>&</sup>lt;sup>8</sup> Mathematica is a registered trademark of Wolfram Research, Inc.

safety software. As stated above, the safety software classification involves software failure that could result in the loss of life or serious injury, exposure to hazardous materials in excess of standards, serious damage to the environment, or noncompliance with laws or regulations.

Excel or other Utility Calculation analyses that are not used for a significant part of a client deliverable, or are only used to double-check analyses, are exempt from these instructions. These instructions apply to the use of scripts and/or macros, within Excel, as well as Excel basic calculations. Portions of this project that have been identified as containing safety software must follow the utility calculations guidance in the SBMS subject area, "Safety Software" (PNNL 2007f). For additional information, refer to the SBMS subject area, "Software," Section 7, "Using Software to Conduct Analyses" (PNNL 2007h).

**NOTE**: Excel is used as the example in these instructions; however, the process is the same for all other Utility Calculations.

These requirements and instructions apply to Project Managers and staff who will use Excel to conduct analysis to be delivered to the client, or to conduct analyses in support of a deliverable to the client. The process shall be implemented as follows:

- <u>Requirements and Risk Identification</u>: Plan out the analysis that will be performed and assess the risk associated with software failure. Document the associated risk and the analysis to be performed (this could be one paragraph in a Microsoft Word<sup>®</sup> document or on another tab in the Excel spreadsheet itself). (See risk examples in Table 17.1.)
- <u>Design and Validation Planning</u>: Prepare and document how the Excel file will be validated, reviewed, and tested by an independent technical reviewer. Identify and document who will perform the independent technical review. (Identify what the problem is that is trying to be solved and what actual calculations are being performed to solve the problem. This information will be useful for the independent technical reviewer. This could be one paragraph in a Word document or on another tab in the Excel spreadsheet.)
- <u>Implementation</u>: Conduct the analysis using the Excel spreadsheet with the appropriate calculations based on the planning previously performed. (If implementation of the analysis has changed, go back and update the risk associated with the analysis and the documentation to be used for the validation, if applicable.)
- <u>Verification</u>: Review and verify the results of the analysis. Review the results produced from the analysis. Determine if the analysis and results support the problem that is trying to be solved. Document the verification and review step. (Documenting this step can be done with one paragraph, in a Word document or on another tab in the Excel spreadsheet, of what was reviewed and identify if the outcome was acceptable or if additional work needs to be done.
- <u>Validation</u>: Conduct independent review of results and validation. Provide the identified independent technical reviewer the Excel spreadsheet and Word document, if applicable. (The reviewer also needs to have all the information regarding the requirements, risk, design and review expectations to perform the review.)

| Identified Risk   | Overall Risk<br>to Project | Preventive Action  | Contingency<br>Action   | Trigger  | Owner                 |
|---|----------------------------|--|---|--|-----------------------|
| Changing<br>requirements<br>after starting<br>design/<br>development                              | Medium                     | Customer approval of<br>requirements before<br>design/ development,<br>flexible design, and<br>configuration<br>management process | Changes affect<br>either schedule or<br>resource allocation                               | Customer<br>request  | Battelle/<br>customer |
| Incomplete input<br>data  | High                       | Identify appropriate<br>sources of validation<br>data  | Manual updates to<br>input tables are<br>tracked through<br>the change control<br>process | Appropriate<br>input tables<br>not available   | Battelle/<br>customer |
| Change in project<br>budget or/or<br>schedule   | Low                        | Define and implement<br>new process  | Continue current process  | Coordinate<br>issues with<br>customer  | Battelle/<br>customer |
| Invalid<br>regulatory<br>products that rely<br>on calculations<br>performed with<br>this software | Low                        | Development and<br>execution of a<br>software test plan to<br>cover all calculations<br>in the system                              | Identify critical<br>calculations and<br>tests based on use<br>of the system              | Software<br>codes are<br>required to be<br>reviewed with<br>a customer<br>QA/quality<br>control<br>process | Customer              |

Overall risk rating is *medium*.

- <u>Independent Technical Review</u>: Reviewer performs the review, per the instructions provided, and <u>documents</u> any additional checks performed on the file that extended outside the original scope of the review and the method used to perform the review of the results. The reviewer <u>documents</u> the outcome of the review. (The documentation can be one paragraph in a Word document or on another tab in the Excel spreadsheet.)
  - The results shall be determined based on using an alternate method to perform the analysis.
    Typical alternate methods include literature review, empirical data, hand-calculations, and executing the analysis on a comparable but different tool.
- <u>Documentation</u>: Print the Excel spreadsheet with the analysis/results and attach the Word document or the tab in the Excel spreadsheet that contains the identified requirements, risk, design, validation steps, verification and independent technical review steps and results. Have the independent technical reviewer sign the document. The verifier needs to sign the verification step. Place this signed document in project records.

### 17.4 Project-Specific Software Requirements

The following subsections apply to researchers participating in the Rifle IFC Site Project who are not PNNL employees, or are engaged in software or computer model development at PNNL or the Hanford Site. If the Idaho National Laboratory (INL) develops the database system for this project, the requirements in the following subsection shall apply to that task.

#### 17.4.1 GEMS and SOARS

GEMS is used by the DOE LM, Grand Junction Project Office, to house and display validated geochemical data for UMTRA Sites. GEMS has been approved by DOE LM for this purpose and the Rifle IFC Site Project accepts this approval as an indication that the GEMS software meets the NQA-1 status of the DOE LM work at UMTRA sites. Currently, the Rifle Project uses GEMS data for overall historical and background assessment of processes operating at the Old Rifle UMTRA site. GEMS does not include data from or apply to the experimental results from the Rifle IFC or past DOE SC BER-funded field research at the site. It is possible the Rifle IFC Site Project will use a special version of GEMS to make Rifle IFC field experimental data available to researchers and perhaps eventually to the public. If this is done, the safety software status will be evaluated in detail before using GEMS in this manner. The GEMS website is located at: <u>http://gems.lm.doe.gov/imf/ext/gems/jsp/launch.jsp</u>.

SOARS (System Operation and Analysis at Remote Sites) is used by DOE LM to capture and archive data collected remotely via sensors at UMTRA sites (<u>https://vdv.gjo.doe.gov/vdv/index.php</u> [password protected]). Similar to the situation for GEMS, the Rifle IFC Site Project accepts the operational and QA status of SOARS in accordance with DOE LM's use of it as commercial software that meets or exceeds all DOE LM QA requirements for UMTRA site work. SOARS is created and maintained by Vista Data Systems (<u>http://www.vistadatavision.com/index.html</u>) and implemented for DOE LM by S.M. Stoller. Dr. Stan Morrison is the SOARS operation contact for DOE LM.

#### 17.4.2 Idaho National Laboratory

Currently, the INL is not part of the Rifle IFC Site Project. However, INL is applying its database and geophysical analysis software to the 300 Area IFC Project. If this software proves to be appropriate for the Rifle IFC Site Project, the INL may be asked to transfer its software to the Rifle IFC via a subcontract revision. If this occurs, INL researchers shall conduct work under this project in accordance with a QA Project Plan based on QA requirements of DOE Order 414.1C, "Quality Assurance," for all software development and use of existing software activities in support of this project.

INL researchers shall establish and perform work processes for developing and using safety software, as defined in DOE Order 414.1C. Work processes involving safety software must be developed and implemented using national or international consensus standards and shall include the following elements:

- Facility design authority involvement in the identification of software requirements specification, acquisition, design, development, verification and validation (including inspection and testing), configuration management, maintenance, and retirement.
- Identify, document, and maintain a safety software inventory.

- Establish grading levels for safety software. Document those grading levels in the QA manual.
- Using the grading levels established and approved in the preceding paragraphs, select and implement applicable software QA work activities from the following list to ensure the safety software performs its intended functions. The American Society of Mechanical Engineers standard NQA-1-2000 shall be used to implement these work activities.
  - Software project management and quality planning
  - Software risk management
  - Software configuration management
  - Procurement and supplier management
  - Software requirements and identification and management
  - Software design and implementation
  - Software safety
  - Verification and validation
  - Problem reporting and corrective action
  - Training of personnel in the design, development, use, and evaluation of safety software.
- These requirements shall be passed to any subcontractors performing work regarding safety software development or use in support of this contract.

A pre-award evaluation shall be conducted of the INL's software development capability and/or usage practices to confirm that it complies with DOE Order 414.1C. Additional audits/assessments of the software development process may be conducted during the project.

### 17.4.3 DOE National Laboratory and University Collaborator Computer Modeling Activities

For all software used in preparation of deliverables for this project, DOE national laboratory and university researchers shall conduct work under their subcontracts in accordance with the following (this includes existing software applications and/or models, and use of spreadsheets for complex calculations):

- <u>Verify the software is applicable to the problem for which it is being used to solve</u>. Document the software used and rational for choosing the application when reporting data calculations from a software application, and which is part of any deliverable for this contract.
- <u>Maintain configuration management of the software used</u>. Identify and document what software is being used for data calculations, what version of the software was used, and what operating system the software was running on when data and/or calculations were produced. This applies when reporting data from a software application that will be part of the deliverables for this contract.
- <u>Validate that the software performs correctly over the range of problems that will be analyzed in performance of the contract.</u>

- Define and document test cases or items to be tested based on what parts of the application are being used. (Identify and document option settings of models used, if applicable.)
- Identify and document, if applicable, values required for input.
- Identify and document acceptance criteria defining the degree of variability that is acceptable between the results of the analysis and results from an alternate method. This could range from exact duplication of the results, to several significant figures, to order of magnitude agreements depending on expectations. Acceptable alternate methods are literature review, empirical data, hand-calculations and/or executing the scenarios on a comparable but different tool. Alternate methods used for acceptance criteria shall be referenced and sources cited.
- Determine method to manage multiple sets of results if the analyses or a portion of the analyses needs to be reproduced or re-executed, when applicable.
- If more than one version of the software will be used to conduct the analyses, determine and document methods for controlling the versions and confirming that the results are consistent across all versions used.
- Conduct the validation according to the cases and items identified. Document the results of the validation, who performed the validation, and when the validation was performed.
- Resolve any bugs and/or problems with the implementation of the software application and revalidate, when necessary, until the results are acceptable. Document and report any outstanding bugs or problems found during validation, and which will not be resolved prior to submitting deliverables.
- <u>An independent reviewer shall verify that the results are accurate either through review or alternate methods of performing the calculations or analysis</u>. Identify and document the independent reviewer, what method was used to verify the results, and if the results and validation of the software application are acceptable.

Requests for and reviews of the documentation in support of the software use may be conducted by PNNL at any time during the project.

# **18.0** Nonconformances and Deficiencies

Procured materials found to be in nonconformance with specifications or where the quality of an activity is found not to be in compliance, the quality problem will be documented in the ATS in accordance with the SBMS subject area, "Quality Problem Reporting" (PNNL 2005c). Corrective actions are documented in the ATS in accordance with the SBMS subject area, "Assessment Management" (PNNL 2005a).

If a deficiency is found where a procedure or process is not followed or the activity is not in compliance with a procedure or process, the deficiency will be documented in the ATS in accordance with the SBMS subject area, "<u>Quality Problem Reporting</u>" (PNNL 2005c). Corrective action will be documented using ATS in accordance with the SBMS subject area, "<u>Assessment Management</u>" (PNNL 2005a) and as discussed in Sections 8.0 and 12.0.

When the analytical data (hard copy or electronic data) are found to be incomplete or deficient in data by the data-processing staff verification, a Problem and Discrepancies Form is filled out in accordance with the PNNL internal procedure DM-3, "Verification of Analytical Data." When the technical staff performs the initial data review and/or a comparison of the recent data to historical trends, any suspect data are submitted to the verification group by a remedial design report in accordance with the project internal procedure DA-3, *Data Review Procedure*. If there are any limitations noted on the data, a flag will be added to the data in spreadsheets or data sets.

Subcontractors will be required to have a system to identify and dispose of nonconforming items, procedure deficiencies, processes not followed, or activities not in compliance to a procedure or a process. This requirement will be specified in a SOW.

## **19.0 Document Control**

#### **19.1 Project Quality Assurance Plan Control**

Distribution and control of this QAPjP shall be performed in accordance with the SBMS subject area, "<u>Publishing Scientific and Technical Information</u>" (PNNL 2007d). Modifications to this plan shall be made either by revision or by issuing an Interim Change Notice (ICN) (see Figure 19.1 for the ICN Form and instructions). This plan will be revised after four ICNs or a major change in project scope or requirements. Any PNNL or Rifle IFC Site Project staff member may request a change to this QAPjP by submitting the requested change in writing to the Project Manager and Quality Engineer. All reviewers listed on the signature page and affected by the change will approve the revision. The ICN will be placed in front of the signature page and the individual pages will be placed or the necessary correction will be lined out and correction added with initial and date. The QAPjP will be reviewed at least annually unless a different review cycle is documented. The current version will reside on the Rifle IFC Site Project SharePoint website.

#### **19.2** Technical Procedure Control

Technical procedures referenced by this QAPjP and used by Rifle IFC Site Project staff will be contained in a PNNL internal procedure manual, or other procedure manual, as appropriate. Technical procedures will be distributed and controlled in accordance with SBMS subject area, "Document Control" (PNNL 2006a). Modifications to any of the internal procedures shall be made either by revision or by issuance of an ICN. The current revisions will be made available as password-protected PDFs on the Rifle IFC Site Project SharePoint website. Procedures will be revised after two major ICNs or if the procedure format has changed. Any PNNL staff member may request a change to procedures at any time by submitting the requested change in writing to the author. The author, technical reviewer, Task Manager, and project Quality Engineer will review and approve the ICN. The Project Manager may

delegate his/her review and approval authority. The ICN will be placed in front of the signature page and the individual affected pages will be included or the necessary correction will be lined out, and the correction added with initials and date, or by using track changes in Word and creating a password-protected PDF. Contact the project Quality Engineer for an electronic copy of the ICN. New or revised technical procedures, whether they will be included in the internal procedures manual or not, must be developed in accordance with SBMS subject area, "<u>Procedures, Permits, and Other Work Instructions</u>" (PNNL 2004). The procedure owner is required to review the procedure at least every 3 years.

## 19.3 Administrative Procedure/Instruction Preparation and Control

Administrative procedures/instructions used by PNNL staff will be developed, approved, and controlled to ensure consistent application by those staff performing the defined task(s). These procedures/instructions will be developed, approved, and controlled in a manner that has been approved by appropriate project management and the Quality Engineer.

### **19.4** Test Plans and Other Work Documents

Test plans and other work instructions used by PNNL staff will be developed, approved, and controlled to ensure consistent application by those staff performing the defined task(s). These procedures/instructions will be developed, approved, and controlled in a manner that has been approved by appropriate project management and Quality Engineer. Any public distribution of test plans and other plans shall be performed in accordance with SBMS subject area, "Publishing Scientific and Technical Information" (PNNL 2007d).

### 19.5 Field Notebooks and Laboratory Record Books

Field notebooks and LRBs used by PNNL Rifle IFC Site Project staff will be managed, controlled, and reviewed in accordance with the SBMS subject area, "Laboratory Record Books" (PNNL 2000). In particular, the Project Manager shall ensure that all field notebooks and LRBs are reviewed at least twice per year. The reviewer, a qualified individual, confirms that there is sufficient detail to trace the investigation and confirm the test results or repeat the investigation and achieve comparable results, without recourse to the original investigator.

| INSTRUCTIONS FOR ICN FORM  |
|--|
| HEADER:  |
| The ICN number is identified as ICN No   |
| For a published document, each page of the ICN shall have a header on the right upper-corner that includes the report number, the date and the pagination. The number of the ICN must be placed after the PNNL number. The second line of the header should show the date and pagination. The cover sheet needs to identify how many pages in the ICN packet.<br>Example header: PNNL-xxxxx-ICN-x<br>Month, day, year; Page x of xx  |
| SECTION A.   |
| Self-explanatory.  |
| SECTION B.   |
| Include all actions that the document holder must take to update the procedure or instruction. Possible actions include: replacing pages of the document with pages that are distributed with the ICN and marking up the document (in ink) to reflect the changes identified on the ICN, or attach the ICN cover sheet to the front of the document. For a "Published" groundwater monitoring plan, include the following statement: "Attach this ICN to the front of the document, just before the title page." |
| SECTION C.   |
| Identify, by title, all personnel whose job functions will be affected by the change and include a brief description of the effect. If there is no effect on personnel (e.g., the change was made to clarify the intent of the procedure or to correct a typographical error), this block should be marked "N/A."  |
| SECTION D.   |
| State the reason for the change followed by a description of the change (including the affected paragraph, information which is deleted, and the actual wording of any replacement test) for each change included on the ICN.  |
| SECTION E.   |
| The Cognizant Manager shall document the reason for not obtaining original reviewers approval and/or any other decisions that must be documented. Additionally, list the individuals who will receive the document (distribution list).  |
| SECTION F.   |
| Identify type of change and document required approvals.   |
| Figure 19.1. Interim Change Notice (Page 1 of 2)   |

| INTERIM CHANGE NOTICE (ICN)          |                            |                             |   |
|--------------------------------------|----------------------------|-----------------------------|---|
| A. Document No.:                     | <b>Revision No.:</b>       | Implementation              |   |
| Document Title:                      |                            | Date of ICN:/_/             |   |
|                                      |                            |                             |   |
| Document's Original Author:          |                            |                             |   |
|                                      |                            | Change Requested By:        |   |
| B. Action:                           |                            |                             |   |
|                                      |                            |                             |   |
|                                      |                            |                             |   |
|                                      |                            |                             |   |
|                                      |                            |                             |   |
|                                      |                            |                             |   |
| C. Effect of Change:                 |                            |                             |   |
|                                      |                            |                             |   |
|                                      |                            |                             |   |
|                                      |                            |                             |   |
|                                      |                            |                             |   |
| D. Reason for Change/Description     | of Change:                 |                             |   |
|                                      |                            |                             |   |
| Reason for Change:                   |                            |                             |   |
| Description of Change:               |                            |                             |   |
| r · · · · · · · · · · · ·            |                            |                             |   |
|                                      |                            |                             |   |
| E. Document Management Decision      | 15:                        |                             |   |
|                                      |                            |                             |   |
|                                      |                            |                             |   |
|                                      |                            |                             |   |
|                                      |                            |                             |   |
|                                      |                            |                             |   |
| F. Task Manager Approval Signatu     | res (Please Sign and Date) | Type of Change (Check one): | : |
|                                      |                            | Minor Major                 |   |
| L                                    |                            |                             |   |
| Project Quality Engineer Approval: _ |                            | Date:                       | _ |
| Author Anneoval                      |                            | Doto:                       |   |
| Author Approval:                     |                            | Date:                       | _ |
| Other Approvals:                     |                            | Date:                       |   |
|                                      |                            |                             |   |

**Figure 19.1** Interim Change Notice (Page 2 of 2)

Non-PNNL Rifle IFC Site Project staff, such as subcontractors and/or collaborators, shall comply with the following procedural steps regarding laboratory records books, or a Rifle IFC Site Project-approved equivalent.

- 1. Use bound books similar to the LRBs with beige-colored binding used by PNNL.
- 2. The initial LRB custodian shall include the title, author, and period covered on the first page of the book. If the LRB is transferred, the new custodian shall enter their name, location, and date received to the lower portion of the information block.
- 3. If persons other than the custodian make entries, the custodian shall list above or below the information block on the first sheet inside the LRB cover the names of those persons, and obtain sample signature and initials from each.
- 4. Use the following procedure as new project number and project or activities are initiated.
  - Record the starting page, the project or activity title on the second page as a table of contents.
  - Record as the first entry the research activity title, the project or work authorization number, and a brief description of the objectives and planned approach.
  - Record observations/data chronologically. Describe (narrative or sketch) experimental apparatus, equipment, and any procedures, data sheets, etc., that are used.
- 5. Date and sign each page. List person(s) who performed the work.
- 6. Record information only in permanent ink, line-out unused portions of pages, and keep pages intact.
- 7. Do not erase or obliterate entries. Mark out errors or corrections with single lines. Initial and date all changes other than editorial corrections. If the change is substantive, record the reason for it.
- 8. Use the following steps if it is necessary to attach a loose sheet.
  - Attach the sheet to an unused page of the LRB by tape or glue.
  - Write the LRB number and the record book page number on the attached sheet (in case it comes loose).
  - Make an entry in the LRB to introduce or describe the attached sheet.
- 9. Maintain a list in the project or activity file identifying the LRB numbers, custodians, and record book locations.
- 10. Record as the last entry for a project or activity a statement noting completion of the work or, if appropriate, reference to a subsequent LRB.
- 11. Store LRBs in metal file cabinets or receptacles that prevent physical damage or access by unauthorized persons when not in use, and allow easy retrieval for periodic inventory.
- 12. Return LRBs to the Rifle IFC Site Project Document Control or Project Manager when complete or at project end. Users may copy appropriate pages for their personal files and future reference.

If the staff member for future reference retains LRBs, they must be protected from physical damage or access by unauthorized persons and made available for periodic inventory.

13. Make copies of LRBs, or applicable pages, for inclusion in project files, when appropriate.

## 20.0 References

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10 CFR 830, Subpart A, "Quality Assurance Requirements." U.S. Code of Federal Regulations.

40 CFR 136, Chapter 1, Appendix B (7/1/01). U.S. Environmental Protection Agency. "Guidelines Establishing Test Procedures for the Analysis of Pollutants." U.S. Code of Federal Regulations.

61 FR 67325-67326. "Final Programmatic Environmental Impact Statement for the Uranium Mill Tailings Remedial Action Ground Water Project." *Federal Register*.

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Appendix A Rifle IFC Site Project Quality Control Plan

# Appendix A Rifle IFC Site Project Quality Control Plan

## A.1 Introduction

This appendix describes the basic methods and procedures to implement **groundwater monitoring** quality control for sampling and analysis conducted in association with the Rifle Integrated Field-Scale (IFC) Site Project. The quality control practices described in this plan help to evaluate whether samples free of contamination are obtained during sampling, and that the laboratory performed sample analyses within the accuracy and precision limits required by the project.

Most information in this appendix applies only to groundwater samplers. Quality control practices and requirements that pertain to soil and sediment samples are described in Section A.5.

The primary objectives of this plan are listed below:

- 1. Identify the quality control elements selected for the Rifle IFC Site Project.
- 2. Provide data quality objectives (DQO) for reporting limits, precision, accuracy, and completeness.
- 3. Indicate actions that are to be taken for out of tolerance data.

## A.2 Technical Requirements

The technical requirements for quality control are divided into two types – components that provide checks on field and laboratory activities (field quality control) and factors that help monitor laboratory performance (laboratory quality control). Each type of quality control sample has required frequencies and acceptance criteria.

The following guidance documents were used as aids in determining the quality control elements necessary for the Groundwater Performance Assessment Project:

- 1. Quality Assurance Manual for the Waste Management Branch Investigations (EPA 910/9-86-00)
- 2. Resource Conservation and Recovery Act (RCRA) Groundwater Monitoring Technical Enforcement Guidance Document (EPA/OSWER-9950.1)
- 3. Test Methods for Evaluating Solid Waste: Physical/Chemical Methods, SW-846, Third Edition (EPA/SW-846, as amended)
- 4. *Handbook for Analytical Quality Control in Water and Wastewater Laboratories* (EPA-600/4-79-019).

Quality control elements were selected based on the needs of the project and the value the results from each type of sample will add to the data.

### A.2.1 Field Quality Control

To indicate whether groundwater samples are collected in a consistent manner and are properly preserved and transported to the analytical laboratory, four types of quality control samples are collected before or during sampling:

- 1. **Full Trip Blanks (FTB)** These samples are prepared by the sampling team before traveling to a sampling site. A preserved bottle set, identical to the set that will be used for sample collection in the field, is filled with reagent water (carbon free, deionized water). The FTB bottles are sealed by the sampling team and transported unopened to the field in the same storage container that will be used for the samples collected that day. These samples are typically analyzed for the same constituents as the samples from the associated well.
- 2. Equipment Blanks (EB) Reagent water is passed through the pump or manifold after decontamination (sometimes just prior to sampling) to collect blank samples identical to a set that will be collected in the field. Preserved bottles are used. The EB bottles are placed in the same container as the associated field samples. EB samples are not removed from the container until delivery to the analytical laboratory.
- 3. Field Duplicates (DUP) A replicate sample that is collected at one well. After each type of bottle is filled, a second, identical bottle is filled for each type of analysis as directed by chain-of-custody requirements. Both sets of samples are stored and transported together.

Using several types of field blank samples provides checks on bottle cleanliness, purity preservation, equipment decontamination, proper storage and transport of samples, and reveals whether or not samples collected for volatiles may have been contaminated during collection. Sampling in replicate provides information about sampling reproducibility. Field quality control sample frequencies are shown in Table A.1. In addition to the evaluation characteristics described in Table A.1, the field quality control samples also provide a check on the analytical laboratory. The field quality control data are designed to give an overall impression of the performance of the sampling and analysis of the PNNL Groundwater Performance Assessment Project; however, individual data points associated with field quality control samples that are outside of the acceptance criteria are flagged in the Rifle IFC Site Project database.
| Field Quality Control   |   |                          |  |  |  |
|---|---|--------------------------|--|--|--|
| Sample Type   | TypePrimary Characteristics EvaluatedFrequency  |                          |  |  |  |
| FTB   | Contamination from containers or transportation | 1 per 20 well trips      |  |  |  |
| EB  | Contamination from non-dedicated equipment      | As needed <sup>(a)</sup> |  |  |  |
| Replicate/duplicate samples   | Reproducibility                                 | 1 per 20 well trips      |  |  |  |
|   | Laboratory Quality Control                      |                          |  |  |  |
| Sample Type   | Primary Characteristics Evaluated               | Frequency                |  |  |  |
| Method blanks   | Laboratory contamination                        | 1 per batch              |  |  |  |
| Lab duplicates  | Laboratory reproducibility                      | (b)                      |  |  |  |
| Matrix spikes   | Matrix effect and laboratory accuracy           | (b)                      |  |  |  |
| Matrix spike duplicates   | Laboratory reproducibility/accuracy             | (b)                      |  |  |  |
| Surrogates  | Recovery/yield                                  | (b)                      |  |  |  |
| Laboratory control samples  | Method accuracy                                 | 1 per batch              |  |  |  |
| <ul> <li>(a) For portable peristaltic pumps, EBs are collected once per 30 well trips. Whenever a new type of non-dedicated equipment is used, an EB shall be collected every time sampling occurs until it can be shown that less-frequent collection of EBs is adequate to monitor the decontamination procedure for the non-dedicated equipment.</li> <li>(b) As defined in the laboratory contract, QA plan, and/or analysis procedures.</li> <li>EB = Equipment blank.</li> <li>FTB = Full-trip blank.</li> <li>QA = Quality assurance.</li> </ul> |   |                          |  |  |  |

## Table A.1. Quality Control Samples

The results of each type of field quality control sample are evaluated according to criteria defined in Table A.2.

| Table A.2. Fie | eld and Laboratory Quality | Control Elements and A | Acceptance Criteria |
|----------------|----------------------------|------------------------|---------------------|
|----------------|----------------------------|------------------------|---------------------|

| метнор  | QUALITY<br>CONTROL<br>ELEMENT | ACCEPTANCE<br>CRITERIA          | CORRECTIVE<br>ACTION         |
|---|-------------------------------|---------------------------------|------------------------------|
| Gen   | eral Chemical Par             | ameters                         |                              |
| Alkalinity - EPA 600 Series, 310.1  | MB <sup>(a)</sup>             | < MDL                           | Flagged with "C"             |
| Chemical Oxygen Demand - EPA 600 Series, 410.4                              | LCS                           | 80-120% recovery <sup>(b)</sup> | Data reviewed <sup>(c)</sup> |
| Conductivity - EPA 600 Series, 120.1  | DUP                           | $\pm 20\% \text{ RPD}^{(b)}$    | Data reviewed <sup>(c)</sup> |
| Oil and Grease - EPA 600 Series, 413.1                                      | MS <sup>(d)</sup>             | 75-125% recovery <sup>(b)</sup> | Flagged with "N"             |
| pH - EPA 600 Series, 150.1  | EB, FTB                       | < 2X MDL                        | Flagged with "Q"             |
| Total Dissolved Solids - EPA 600 Series, 160.1                              | Field Duplicate               | $\pm 20\% \text{ RPD}^{(e)}$    | Flagged with "Q"             |
| Total Organic Carbon - SW-846, 9060<br>Total Organic Halides - SW-846, 9020 |                               |                                 |                              |
|   | Ammonia and An                | ions                            |                              |
| Ammonia - EPA 600 Series, 350.1   | MB                            | < MDL                           | Flagged with "C"             |
| Anions by IC - EPA 600 Series, 300.0  | LCS                           | 80-120% recovery <sup>(b)</sup> | Data reviewed <sup>(c)</sup> |
| Cyanide - SW-846, 9012  | DUP                           | $\pm 20\% \text{ RPD}^{(b)}$    | Data reviewed <sup>(c)</sup> |
|   | MS                            | 75-125% recovery <sup>(b)</sup> | Flagged with "N"             |

| METHOD   | QUALITY<br>CONTROL<br>ELEMENT | ACCEPTANCE<br>CRITERIA                               | CORRECTIVE<br>ACTION         |  |  |
|--|-------------------------------|--|------------------------------|--|--|
|  | EB, FTB                       | < 2X MDL   | Flagged with "Q"             |  |  |
|  | Field Duplicate               | $\pm 20\% \text{ RPD}^{(e)}$                         | Flagged with "Q"             |  |  |
| Metals   |                               |  |                              |  |  |
| Arsenic - SW-846, 7060   | MB                            | < CRDL   | Flagged with "C"             |  |  |
| Cadmium - SW-846, 7131   | LCS                           | 80-120% recovery <sup>(b)</sup>                      | Data reviewed <sup>(c)</sup> |  |  |
| Chromium - SW-846, 7191  | MS                            | 75-125% recovery <sup>(b)</sup>                      | Flagged with "N"             |  |  |
| Lead - SW-846, 7421  | MSD                           | $\pm 20\% \text{ RPD}^{(b)}$                         | Data reviewed <sup>(c)</sup> |  |  |
| Mercury - SW-846, 7470   | EB, FTB                       | < 2X MDL   | Flagged with "Q"             |  |  |
| Selenium - SW-846, 7740  | Field Duplicate               | $\pm 20\% \text{ RPD}^{(e)}$                         | Flagged with "Q"             |  |  |
| Thallium - SW-846, 7841<br>ICP Metals - SW-846, 6010   |                               |  |                              |  |  |
| ICP/MS Metals - SW-846, 6010<br>ICP/MS Metals - SW-846, 6020   |                               |  |                              |  |  |
|  | <br>Radiological Param        | ators  |                              |  |  |
| Gamma Scan   | MB                            | < 2X MDA   | Flagged with "B"             |  |  |
| Gross Alpha - SW-846, 9310   | LCS                           | 70-130% recovery                                     |                              |  |  |
| Gross Beta - SW-846, 9310  | DUP                           | $\pm 20\%$ RPD                                       | Data reviewed <sup>(c)</sup> |  |  |
| Iodine-129   | MS <sup>(h)</sup>             |  |                              |  |  |
|  |                               | 60-140% recovery                                     |                              |  |  |
| Plutonium (isotopic)   | EB, FTB                       | $\frac{<2X \text{ MDA}}{\pm 20\% \text{ RPD}^{(5)}}$ | Flagged with "Q"             |  |  |
| Strontium-89/90  | Field Duplicate               | $\pm 20\%$ RPD <sup>(*)</sup>                        | Flagged with "Q"             |  |  |
| Technetium-99  |                               |  |                              |  |  |
| Tritium - SW-846, 906.0  |                               |  |                              |  |  |
| Tritium (low-level)<br>Uranium (isotopic)  |                               |  |                              |  |  |
| Uranium (total)  |                               |  |                              |  |  |
| ~ /  |                               |  |                              |  |  |
| <ul> <li>(a) Does not apply to pH.</li> <li>(b) Laboratory-determined, statistically derived control limits may also be used. Such limits are reported with the data.</li> <li>(c) After review, corrective actions are determined on a case-by-case basis. Corrective actions may include a laboratory recheck or flagging the data as suspect (Y flag) or rejected (R flag).</li> <li>(d) Applies to total organic carbon and total organic halides only.</li> <li>(e) Applies to total organic carbon and total organic halides only.</li> <li>(e) Applies to total organic carbon and total organic halides only.</li> <li>(f) Determined by the laboratory based on historical data. Control limits are reported with the data.</li> <li>(g) For common laboratory contaminants such as acetone, methylene chloride, 2-butanone, toluene, and phthalate esters, the acceptance criteria is &lt;5 times MDL.</li> <li>(h) Applies only to technetium-99 and total uranium analyses.</li> <li>Data Flags:</li> <li>B, C = Possible laboratory contamination (analyte was detected in the associated method blank).</li> <li>N = Result may be biased (associated matrix spike result was outside the acceptance limits).</li> <li>Q = Problem with associated field quality control sample (blank and/or duplicate results were out of limits).</li> <li>DUP = Laboratory matrix duplicate.</li> <li>EB = Equipment blank.</li> <li>FTB = Full trip blank.</li> <li>FXR = Field transfer blank.</li> <li>GC = Gas chromatography.</li> <li>ICP = Inductively coupled plasma.</li> <li>ICP/MS = Inductively coupled plasma.</li> <li>ICP/MS = Inductively coupled plasma.</li> <li>ICP/MS = Inductively coupled plasma.</li> <li>MB = Method blank.</li> </ul> |                               |  |                              |  |  |

|      | METHOD                         | QUALITY<br>CONTROL<br>ELEMENT | ACCEPTANCE<br>CRITERIA | CORRECTIVE<br>ACTION |
|------|--------------------------------|-------------------------------|------------------------|----------------------|
| MDA  | = Minimum detectable activity. |                               |                        |                      |
| MDL  | = Method detection limit.      |                               |                        |                      |
| MS   | = Matrix spike.                |                               |                        |                      |
| MSD  | = Matrix spike duplicate.      |                               |                        |                      |
| PCBs | = Polychlorinated biphenyls.   |                               |                        |                      |
| RPD  | = Relative percent difference. |                               |                        |                      |
| SUR  | = Surrogate.                   |                               |                        |                      |

Bias is assessed by comparing a measured value to a known or accepted reference value or the recovery of a known amount of spiked contaminant into a sample (i.e., a matrix spike [MS]). An MS bias caused by matrix effects is calculated in Equation (A.1):

$$\mathbf{B} = (\mathbf{X}_{\mathrm{s}} - \mathbf{X}_{\mathrm{u}}) - \mathbf{K} \tag{A.1}$$

where

X = measured value of spiked sample

 $X_u$  = sample or miscellaneous contribution

K = known value of spike

Using Equation (A.2) yields percent recovery (%R):

$$%R = 100 (X_s - X_u) / K$$
 (A.2)

Analytical precision is determined by analyzing duplicates (field or lab). Precision is expressed as either percent relative standard deviation (RSD) or relative percent difference (RPD). Duplicate results are flagged if the results of both samples are quantifiable (i.e., the result is greater than the 5 times the instrument detection limit [IDL]/method detection limit [MDL]/MDA and the RPD is greater than 20%. The RPD is calculated in Equation (A.3):

$$RPD = \frac{D_1 - D_2}{(D_1 + D_2)/2} \times 100$$
(A.3)

where  $D_1$  = original sample value  $D_2$  = duplicate sample value.

When more than two data values are present, calculate precision by the RSD (Equation [A.4]):

$$RSD = \frac{\text{standard deviation}}{\text{mean}} \times 100$$
(A.4)

#### A.2.2 Quality Control in the Laboratory

The ability of the laboratories to perform sample analyses within the limits established by the project is monitored in several ways. Internal quality assurance programs are maintained by laboratories participating in the Rifle IFC Site Project. In addition, the laboratories are periodically reviewed and audited both internally and externally. PNNL participates in external audits. Laboratory quality

assurance includes a comprehensive quality control program, which includes the use of MS, matrix duplicates (MD), matrix spike duplicates (MSD), laboratory control samples (LCS), surrogates, tracers, and blanks. These samples are recommended in the guidance documents and are required by U.S. Environmental Protection Agency (EPA) protocol.

**Matrix Duplicate** — An intra-laboratory split sample that is used to evaluate the precision of a method in a given sample matrix.

**Matrix Spike** — An aliquot of a sample spiked with a known concentration of target analyte(s). The MS is used to assess the bias of a method in a given sample matrix. Spiking occurs prior to sample preparation and analysis.

**Matrix Spike Duplicate** — A replicate spiked aliquot of a sample that is subjected to the entire sample preparation and analytical process. MSD results are used to determine the bias and precision of a method in a given sample matrix.

**Laboratory Control Sample** — A control matrix spike (e.g., deionized water) spiked with analytes representative of the target analytes or a certified reference material that is used to evaluate laboratory accuracy.

**Method Blank** — An analyte-free matrix to which all reagents are added in the same volumes or proportions as used in sample processing. The method blank is carried through the complete sample preparations and analytical procedure. The method blank is used to quantify contamination resulting from the analytical process.

**Surrogates** — A compound added to all samples in the analysis batch (field samples and quality control samples) prior to preparation. The surrogate is typically similar in chemical composition to the compound or analyte being determined, yet not normally encountered in most samples. Surrogates are expected to respond to the preparation and measurement systems in a manner similar to the analytes of interest. Because surrogates are added to all standards, samples, and quality control samples, they are a useful tool in evaluating overall method performance in a given matrix. Surrogates are utilized only in organic analyses.

**Tracers** — A tracer is a known quantity of radioactive isotope that is different from that of the isotope of interest but is expected to behave similarly and is added to an aliquot of sample. Sample results are generally corrected based on tracer recovery.

The laboratories are required to analyze samples within the holding times specified by the analysis procedure. In some instances, constituents in samples not analyzed within the holding time may be compromised by volatilization, decomposition, or other chemical changes. Data from samples analyzed outside the holding time are flagged in the Rifle IFC Site Project database with an "H." The holding times for constituents analyzed by the Rifle IFC Site Project are listed in Table A.3.

| Constituents                | Methods <sup>(a)</sup> | Holding Times |
|-----------------------------|------------------------|---------------|
| ICP metals                  | SW-846, 6010           | 6 months      |
| ICP-MS                      | SW-846, 6020           | 6 months      |
| Arsenic                     | SW-846, 7060           | 6 months      |
| Lead                        | SW-846, 7421           | 6 months      |
| Mercury                     | SW-846, 7470/7471      | 28 days       |
| Selenium                    | SW-846, 7740           | 6 months      |
| Thallium                    | SW-846, 7841           | 6 months      |
| Alkalinity                  | EPA 600 Series, 310.1  | 14 days       |
| Cyanide                     | SW-846, 9010/9012      | 14 days       |
| Bromide                     | EPA 600 Series, 300.0  | 28 days       |
| Chloride                    | EPA 600 Series, 300.0  | 28 days       |
| Fluoride                    | EPA 600 Series, 300.0  | 28 days       |
| Nitrate                     | EPA 600 Series, 300.0  | 48 hours      |
| Nitrite                     | EPA 600 Series, 300.0  | 48 hours      |
| Phosphate                   | EPA 600 Series, 300.0  | 48 hours      |
| Sulfate                     | EPA 600 Series, 300.0  | 28 days       |
| Total organic carbon        | SW-846, 9060           | 28 days       |
| Total organic halides       | SW-846, 9020           | 28 days       |
| Chemical oxygen demand      | EPA 600 Series, 410.4  | 28 days       |
| (a) EPA/SW-846, as amended. |                        |               |

 Table A.3.
 Rifle IFC Site Project Holding Times

Other tools are used by the project to evaluate the laboratories. Double-blind standards of the constituents of concern are submitted to the primary laboratory in triplicate or quadruplicate on a quarterly basis. Because the results of double-blind standards provide information on laboratory precision and accuracy, these standards are useful tools to verify project DQOs are being met. Table A.4 lists the typical blind-standard constituents and their submission frequencies. Due to the occasional need to investigate potential problems at the laboratories, the list of constituents is subject to change. Specific information about the constituents used and their spiking levels will be maintained in the project files.

| Constituents                         | Frequency         | Recommended Recovery<br>(%) <sup>(a)</sup> | Precision (%RSD) <sup>(a)</sup>      |
|--------------------------------------|-------------------|--|--------------------------------------|
| Fluoride                             | Quarterly         | ±25%                                       | ±25%                                 |
| Nitrate                              | Quarterly         | ±25%                                       | ±25%                                 |
| Cyanide                              | Quarterly         | ±25%                                       | ±25%                                 |
| Chromium                             | Annually          | ±20%                                       | ±20%                                 |
| Total organic carbon <sup>(b)</sup>  | Quarterly         | Varies according to spiking compound       | Varies according to spiking compound |
| Total organic halides <sup>(c)</sup> | Quarterly         | Varies according to spiking compound       | Varies according to spiking compound |
| Gross alpha <sup>(d)</sup>           | Quarterly         | 70 - 130%                                  | ±20%                                 |
| Gross beta <sup>(e)</sup>            | Quarterly         | 70 - 130%                                  | ±20%                                 |
| Tritium                              | Annually          | 70 - 130%                                  | ±20%                                 |
| Tritium (low level)                  | Semi-annual       | 70 - 130%                                  | ±20%                                 |
| Cobalt-60                            | Annually          | 70 - 130%                                  | ±20%                                 |
| Strontium-90                         | Quarterly         | 70 - 130%                                  | ±20%                                 |
| Technetium-99                        | Quarterly         | 70 - 130%                                  | ±20%                                 |
| Iodine-129                           | Semi-<br>annually | 70 - 130%                                  | ±20%                                 |
| Cesium-137                           | Annually          | 70 - 130%                                  | ±20%                                 |
| Uranium                              | Quarterly         | 70 - 130%                                  | ±20%                                 |
| Plutonium-239/240                    | Quarterly         | 70 - 130%                                  | ±20%                                 |

 Table A.4.
 Blind-Standard Constituents and Schedule

(a) If the results are less than 5 times the required detection limit, then the criteria are that the difference of the results of the replicates is less than the required detection limit.

(b) The spiking compound generally used for total organic carbon (TOC) is potassium phthalate. Other spiking compounds may also be used.

(c) Two sets of spikes for total organic halides (TOX) will be used. The spiking compound for one set should be 2,4,5-trichlorophenol. The spiking compound for the second set should include the constituents used for the volatile organic compounds sample (carbon tetrachloride, chloroform, trichloroethylene).

(d) The gross alpha sample will be prepared from Pu-239.

(e) The gross beta sample will be prepared from Sr-90.

RSD = Relative standard deviation.

Blind standards are prepared by spiking matrix groundwater and deionized water with known concentrations of constituents of interest. Spiking concentrations range from MDA or MDL, depending on the constituent measured, to the upper limit of concentration determined in groundwater at the Rifle, Colorado site.

Blind-standard results are evaluated by comparing the laboratory results to the actual spike values. Laboratory precision is also considered as the samples are sent to the laboratory in replicate. Laboratory results are evaluated based on the recovery and precision criteria listed in Table A.4. Results outside of these control limits are investigated and appropriate actions are taken, if necessary.

## A.3 Data Quality Objectives

DQOs are defined for reporting limits, precision, accuracy, and completeness. Groundwater monitoring plans or sampling analysis plans specify whether or not a particular site has more stringent DQOs than those specified in this plan.

Limits for precision and accuracy for chemical analyses are based on criteria stipulated in the methods (e.g., EPA/SW-846, EPA 600 series). Precision and accuracy limits for radiochemical results are specified in the laboratory contract.

Completeness is defined as the percentage of data points judged to be valid. The percent complete each quarter should be at least 85%.

Reporting limits for radiochemical constituents are defined in the laboratory contract. Reporting limits as low as one-third the derived 4-mrem-dose requirement are preferred, but are not always achievable. Preferred reporting limits and actual reporting limits are listed in Table A.5 for radiochemical constituents. For chemical constituents, MDLs as low as one-third the EPA drinking water standards are preferred. In some cases, MDLs that are one-third the regulatory limit are not feasible (e.g., penta-chlorophenol and cadmium). Because MDLs change frequently, these values are not provided in this document.

| Constituent of<br>Concern | Method             | CAS #      | DWS          | One-Third<br>DWS | RDL       |
|---------------------------|--------------------|------------|--------------|------------------|-----------|
| Gross alpha               | Gross alpha - GA   | 12587-46-1 | 15 pCi/L*    | 5 pCi/L*         | 3 pCi/L   |
| Gross beta                | Gross beta - GB    | 12587-47-2 | N/A          | N/A              | 4 pCi/L   |
| Cobalt-60                 | Gamma spec         | 10198-40-0 | 100 pCi/L    | 33 pCi/L         | 25 pCi/L  |
| Cesium-137                |                    | 10045-97-3 | 200 pCi/L    | 67 pCi/L         | 15 pCi/L  |
| Europium-152              |                    |            |              |                  | 50 pCi/L  |
| Europium-154              |                    |            | 200 pCi/L    | 67 pCi/L         | 50 pCi/L  |
| Europium-155              |                    |            | 600 pCi/L    | 200 pCi/L        | 50 pCi/L  |
| Tritium                   | Н-3                | 10028-17-8 | 20,000 pCi/L | 6700 pCi/L       | 400 pCi/L |
| Tritium                   | H-3 (LL)           | N/A        | N/A          | N/A              | 10 pCi/L  |
| Iodine-129                | I-129              | 10043-66-0 | 1 pCi/L      | 0.33 pCi/L       | 5 pCi/L   |
| Iodine-129                | I-129 (LL)         | N/A        | N/A          | N/A              | 1 pCi/L   |
| Strontium-90              | Sr-89/Sr-90        | 10098-97-2 | 8 pCi/L      | 2.7 pCi/L        | 2 pCi/L   |
| Technetium-99             | Тс-99              | 14133-76-7 | 900 pCi/L    | 300 pCi/L        | 15 pCi/L  |
| Plutonium-238             | Isotopic plutonium |            | 1.6 pCi/L    | 0.5 pCi/L        | 1 pCi/L   |
| Plutonium-239/240         | Plutonium-AEA      |            | 1.2 pCi/l    | 0.4 pCi/L        | 1 pCi/L   |
| Uranium-233               | Isotopic uranium   | 13968-55-3 | 20 pCi/L     | 6.7 pCi/L        | 1 pCi/L   |
| Uranium-234               | Isotopic uranium   | 13966-29-5 | 20 pCi/L     | 6.7 pCi/L        | 1 pCi/L   |
| Uranium-235               | Uranium-AEA        | 15117-96-1 | 24 pCi/L     | 8 pCi/L          | 1 pCi/L   |
| Uranium-238               |                    | U-238      | 24 pCi/L     | 8 pCi/L          | 1 pCi/L   |

Table A.5. Reporting Limits for Radiochemical Constituents

| Constituent of<br>Concern                    | Method                                      | CAS # | DWS     | One-Third<br>DWS | RDL      |
|--|---|-------|---------|------------------|----------|
| Total alpha energy<br>emitted from<br>radium | Total radium                                | N/A   | N/A     | N/A              | 1 pCi/L  |
| Uranium<br>(elemental)                       | Total uranium                               | N/A   | 30 µg/L | 10 µg/L          | 0.1 μg/L |
| DWS = Drinking v<br>N/A = Not applied        | abstract service number.<br>water standard. |       |         |                  |          |

### A.4 Reporting and Deliverables Requirements

The results of the blind standards and the field quality control samples will be provided through current analytical reporting procedures. The quality control analytical results will be reviewed by the project staff and compiled in a database for evaluation and reporting.

All project records associated with quality control are maintained in accordance with the Records Inventory and Disposition Schedule for the Rifle IFC Site Project.

### A.5 Requirements for Soil and Sediment Samples

The Rifle IFC Site Project will have soil or sediment samples analyzed in support of site-characterization activities. This work precludes specification of many of the requirements listed previously for groundwater samples. Therefore, the types, quantities, and acceptance criteria for field and/or laboratory quality control samples are specified in test plans. Table A.6 lists the maximum recommended holding times for common analytes in soils. Radionuclides are not included in the table.

| Constituents | <b>Methods</b> <sup>(a)</sup> | Holding Times |
|--------------|-------------------------------|---------------|
| ICP metals   | SW-846, 6010                  | 6 months      |
| ICP-MS       | SW-846, 6020                  | 6 months      |
| Arsenic      | SW-846, 7060                  | 6 months      |
| Lead         | SW-846, 7421                  | 6 months      |
| Mercury      | SW-846, 7470/7471             | 28 days       |
| Selenium     | SW-846, 7740                  | 6 months      |
| Thallium     | SW-846, 7841                  | 6 months      |
| Alkalinity   | EPA 600 Series, 310.1         | 14 days       |
| Cyanide      | SW-846, 9010/9012             | 14 days       |
| Bromide      | EPA 600 Series, 300.0         | 28 days       |
| Chloride     | EPA 600 Series, 300.0         | 28 days       |
| Fluoride     | EPA 600 Series, 300.0         | 28 days       |

Table A.6. Holding Times for Soil and Sediment Analyses

| Constituents                            | Methods <sup>(a)</sup> | Holding Times |  |
|---|------------------------|---------------|--|
| Nitrate                                 | EPA 600 Series, 300.0  | 48 hours      |  |
| Nitrite                                 | EPA 600 Series, 300.0  | 48 hours      |  |
| Phosphate                               | EPA 600 Series, 300.0  | 48 hours      |  |
| Sulfate                                 | EPA 600 Series, 300.0  | 28 days       |  |
| Total organic carbon                    | SW-846, 9060           | 28 days       |  |
| Total organic halides                   | SW-846, 9020           | 28 days       |  |
| Chemical oxygen demand                  | EPA 600 Series, 410.4  | 28 days       |  |
| (a) EPA/SW-846, as amended (EPA 1986c). |                        |               |  |

## A.6 References

EPA-600/4-79-019. 1979. *Handbook for Analytical Quality Control in Water and Wastewater Laboratories*. U.S. Environmental Protection Agency, Cincinnati, Ohio.

EPA 910/9-86-00. 1986. *Quality Assurance Manual for Waste Management Branch Investigations*. U.S. Environmental Protection Agency, Region 10, Seattle, Washington.

EPA/OWSER-9950.1. 1986. *Resource Conservation and Recovery Act (RCRA) Groundwater Monitoring Technical Enforcement Guidance Document*. U.S. Environmental Protection Agency, Washington, D.C.

EPA/SW-846. 1986, as amended. *Test Methods for Evaluating Solid Waste: Physical/Chemical Methods, SW-846, Third Edition.* Office of Solid Waste and Emergency Response, U.S. Environmental Protection Agency, Washington, D.C. Available online at <a href="http://www.epa.gov/epaoswer/hazwaste/test/sw846.htm">http://www.epa.gov/epaoswer/hazwaste/test/sw846.htm</a>

Appendix B Experimental and Modeling Procedures for the Rifle IFC Site Project

# Appendix B Experimental and Modeling Procedures for the Rifle IFC Site Project

The documents in Table B.1 provide selected procedures, protocols, and references. Given the research nature of the Rifle IFC Site Project, it is expected that additional protocols will need to be developed or adapted from other existing resources (see Appendix C). Additionally, Rifle IFC subcontractors or collaborators typically will have existing published procedures or protocols that can be incorporated into Rifle IFC Site Project procedures.

| Method   | Analysis  | Document Number   | Procedure/Document Title  |
|--|---|---|---|
| Conduct of Routine<br>Laboratory Operations                                  | General   | RPL-OP-001  | "Routine Research<br>Operations,"<br>Section 31, Tab 3 of<br><i>RPL Laboratory Handbook</i>   |
| Inductively Coupled<br>Plasma-Optical Emission<br>Spectroscopy<br>(ICP-OES)* | Ca, K, Mg, P, Sr, Na, Si,<br>Cu, Fe, Mn, S, and Ti in<br>water in ppb or moles/L  | PNNL-AGG-ICP-AES*   | Inductively Couple Plasma –<br>Optical Emission<br>Spectrometry (ICP-OES)<br>Analysis   |
| Inductively Coupled<br>Plasma-Mass<br>Spectroscopy (ICP-MS)                  | Re, Tc  | PNNL-AGG-415  | Inductively Coupled Plasma<br>Mass Spectrometric (ICP-<br>MS) Analysis  |
| Ion Chromatography   | F, Cl, NO <sub>2</sub> , NO <sub>3</sub> , CO <sub>3</sub> ,<br>SO <sub>4</sub> , PO <sub>4</sub> , PO <sub>4</sub> in water<br>in ppm or moles/L | PNNL-AGG-IC-001*  | Determinations by Ion<br>Chromatography (IC)  |
| ICP-MS   | Cu, Fe in water in ppb<br>or moles/L  | PNL-SAND-3.1 (needs to be updated)  | -   |
| КРА  | U in water in ppb or<br>moles/L   | Liu et al. (2004)   | Desorption Kinetics of<br>Radiocesium from<br>Subsurface Sediments at<br>Hanford Site, USA  |
| Spectrophotometer  | Fe(II) and total Fe in ppb  | Kukkadapu et al. (2004)   | Biotransformation of Two-<br>Line Silica-Ferrihydrite by a<br>Dissimilatory Fe(III)-<br>Reducing Bacterium:<br>Formation of Carbonate<br>Green Rust in the Presence of<br>Phosphate |
| LSC  | Sr-90, Tc-99, I-129, in<br>dpm/mL   | PNNL-AGG-RRL-002*;<br>Procedures vary slightly<br>for different<br>radioisotopes; McKinley<br>et al. (2006) for Sr-90 |   |

Table B.1. Rifle IFC Site Project Procedures and Protocols

| Method   | Analysis   | Document Number              | Procedure/Document Title  |
|--|--|------------------------------|---|
| Solid-State pH Electrode and Meter   | pH, Bromide  | AGG-PH-001                   | pH Measurement  |
| X-Ray Diffraction<br>(XRD)   | Mineralogy   | RPL-XRD-PIP                  | Operation of Scintag Pad-V<br>X-Ray Diffractor (RGD #62)  |
| Scanning Electron<br>Microscopy/Energy-<br>Dispersive X-Ray<br>Spectrometry<br>(SEM/EDS) | Particle morphology,<br>size, and qualitative<br>elemental analysis  | PNL-SP-3                     | Scanning Electron<br>Microscopy/ Energy<br>Dispersive Spectrometry  |
| Particle Size Distribution   |  | PNL-MA-567, SA-3             | Particle-Size Analysis<br>(Pipette Or Hydrometer<br>Method); Wet Sieve Analysis<br>Will Be Used To Remove<br>Sand-Size Particle |
| Hydraulic Conductivity   |  | PNL-MA-567, SA-5             | Falling Head Hydraulic<br>Conductivity  |
| Water Retention  |  | UFA-SK-01                    | Determination of Water<br>Retention as a Function of<br>Water Content Using Open-<br>Flow Centrifugation<br>Techniques          |
| Water Content  |  | PNL-MA-567, SA-7             | Water Content   |
| Bulk Density   |  | PNL-MA-567, SA-8             | Clod Density/Bulk Density   |
| Particle Density   |  | PNL-MA-567, SA-9             | Determining Particle Density;<br>Necessary for Constant Head<br>Hydraulic Conductivity  |
| Column Packing   |  | WHC-IP-0635, GEL-3<br>Rev. 3 | Moisture Relationships of<br>Soils; Necessary for Constant<br>Head Hydraulic Conductivity                                       |
| pH/EC  |  | PNL-G-5-pH/EC                | Measuring pH/EC of Low-<br>Level Radioactive Solutions  |
| Saturated Column<br>Experiments  |  | AGG-SAT-COL-001              | Conducting Saturated<br>Column Experiments  |
| Batch Experiments  |  | AGG-BSE-001                  | Batch Sorption Experiments  |
| Surface Area   |  | AGG-SA-001                   | Measuring Surface Area  |
| TIC/TOC  | Inorganic C, organic C,<br>total C   | PNNL-AGG-TOC-001*            |   |
| X-Ray Fluorescence   | Total analyses of<br>sediments including Al,<br>Si, K, Ca, Mg, Sr, Ti,<br>Fe, Mn, Cu, Ni, Cr, Cs,<br>U, and others | PNNL-AGG-OP-<br>RGD74-001*   |   |
| Conventional Powder<br>X-Ray Diffraction   | Mineral identity (% distribution)  | Qafoku et al. 2005           | Kinetic Desorption and<br>Sorption of U(VI) During<br>Reactive Transport in a<br>Contaminated Hanford<br>Sediment               |

| Method  | Analysis   | Document Number  | Procedure/Document Title  |  |  |
|---|--|--|---|--|--|
| Digital Autoradiography   | Identify locations of<br>radioactivity in sediment<br>thin section and<br>mixtures of sand and<br>silt-sized particles.  | Zeissler et al. 2001;<br>McKinley et al. 2001  | Radioactive Particle Analysis<br>by Digital Autoradiography.<br>The Distribution and<br>Retention of <sup>137</sup> Cs in<br>Sediments at the Hanford<br>Site, Washington.  |  |  |
| Scanning Electron<br>Microscopy with WDS  | High-resolution imaging<br>of particle morphology<br>and atomic mass<br>generally in sediment<br>thin section;<br>semiquantitative<br>imaging of chemical<br>distribution. | McKinley et al. 2005   | Precipitation of Waste<br>Uranium as a Uranyl Silicate<br>in Microfractures   |  |  |
| Transmission Electron<br>Microscopy with<br>Selected Area<br>Diffraction (SAED) | Very high resolution of<br>single mineral grains in<br>cross section; local<br>morphology, structure<br>and atomic arrangement.  | Zachara et al. 2006.<br>Selected area diffraction<br>patterns are interpreted<br>using the JADE software<br>(see below) using X-ray<br>powder diffraction data<br>(PDF) retrieved from a<br>standards library (ICDD<br>2003) | Sorption of Cs+ to Micaceous<br>Subsurface Sediments from<br>the Hanford Site, USA  |  |  |
| Electron Microprobe   | Quantitative, interme-<br>diate sensitivity<br>chemical mapping in<br>thin sections. Chemical<br>transects across grain/<br>particle boundaries.                           | Wang et al. 2005b;<br>Catalano et al. 2006   | Cryogenic Laser Induced<br>U(VI) Fluorescence Studies<br>of a U(VI) Substituted<br>Natural Calcite: Implications<br>to U(VI) Speciation in<br>Contaminated Hanford<br>Sediments.  |  |  |
|   |  |  | Changes in Uranium<br>Speciation Through a Depth<br>Sequence of Contaminated<br>Hanford Sediments.  |  |  |
| X-Ray Fluorescence<br>Microprobe  | High sensitivity,<br>semiquantitative<br>mapping of element<br>distributions in sediment<br>thin sections at scales of   | Liu et al. 2004;<br>Fredrickson et al. 2004  | Dissolution of Uranyl<br>Microprecipitates in<br>Subsurface Sediments at<br>Hanford Site, USA.<br>Reduction of TcO <sup>4-</sup> by   |  |  |
|   | 10 μm.   |  | Sediment-Associated<br>Biogenic Fe(II).   |  |  |
| X-Ray Absorption<br>Spectroscopy  | Determination of<br>element coordination<br>structure, nearest<br>neighbors, and bond<br>distances in contami-<br>nated sediment.  | Catalano et al. 2004;<br>Catalano et al. 2006.<br>Basic experimental<br>synchrotron measure-<br>ments are modeled with<br>FEFF, FEFFIT, and<br>IFEFFIT (see below) to<br>extract molecular<br>information.                   | Spectroscopic and Diffraction<br>Study of Uranium Speciation<br>in Contaminated Vadose<br>Zone Sediments from the<br>Hanford Site, Washington<br>State.<br>Changes in Uranium<br>Speciation Through a Depth<br>Sequence of Contaminated<br>Hanford Sediments. |  |  |

| Method  | Analysis  | Document Number  | Procedure/Document Title  |  |  |
|---|---|--|---|--|--|
| Synchrotron Diffraction   | Identification of mineral<br>structures in sediment<br>thin sections.   | Catalano et al. 2004.<br>Mineral structures are<br>derived by application of<br>the FIT2D software (see<br>below).   | Spectroscopic and Diffraction<br>Study of Uranium Speciation<br>in Contaminated Vadose<br>Zone Sediments from the<br>Hanford Site, Washington<br>State  |  |  |
| Cryogenic Laser Induced<br>Fluorescence<br>Spectroscopy (CLIFS) | Vibronic spectra of<br>U(VI) in water and<br>solids to establish<br>molecular and<br>mineralogic<br>environment.  | Wang et al. 2004 (for<br>aqueous solutions); Wang<br>et al. 2005a (for solids).<br>Data analysis is<br>performed using the<br>IGOR and Globals<br>programs (see below).  | Cryogenic Laser Induced<br>Fluorescence<br>Characterization of U(VI) in<br>Hanford Vadose Zone Pore<br>Waters.<br>Fluorescence Spectroscopy of<br>U(VI)-Silicates and U(VI)-<br>Contaminated Hanford<br>Sediment. |  |  |
| Batch Kinetic Desorption<br>Experiments                         | Sediments are bathed in<br>electrolyte of known<br>compositions and the<br>time-variant release of<br>contaminants, and other<br>solid-associated ions are<br>monitored by aqueous<br>phase analyses.   | Procedures vary as per<br>element and its concen-<br>tration. Examples<br>include Liu et al. 2003<br>(Cs-137); Liu et al. 2004<br>(U); McKinley et al. 2005<br>(Sr-90). Kinetic rate laws<br>and rate constants are<br>calculated from the data<br>using microscopic,<br>diffusion based transport<br>models (see below).<br>Steady-state values can<br>be used to establish<br>thermodynamic param-<br>eters, such as the<br>solubility product of a<br>precipitated contaminant<br>phase (e.g., Ilton et al.<br>2006). |   |  |  |
| Batch Adsorption<br>Experiments                                 | Sediments are bathed in<br>electrolytes of a known<br>composition that has<br>been spiked with a<br>contaminant of interest.<br>The adsorption of the<br>contaminant is<br>monitored as a function<br>of pH, ionic strength, or<br>ion composition. | Example procedures are<br>equilibrium – Turner<br>et al. 1996 (U) and<br>Zachara et al. 2002 (Cs);<br>kinetic – Liu et al. 2003<br>(Cs), Liu et al. 2004 (U),<br>and McKinley et al. 2006<br>(Sr). Experimental<br>results are fitted with<br>various geochemical<br>models (MINTEQ;<br>Geochemists Workbench;<br>GMIN; or FITEQL see<br>below) to identify suites<br>of adsorption reactions<br>(ion exchange or surface<br>complexation).  |   |  |  |

| Method                | Analysis   | Document Number  | Procedure/Document Title   |
|-----------------------|--|--|--|
| Column Experiments    | Sediment (<2 mm or<br><4 mm) is packed into a<br>cylindrical plastic, glass,<br>or stainless-steel<br>column. Electrolyte<br>with or without a<br>contaminant tracer is<br>applied to the column to<br>study the release (from<br>contaminated sediment)<br>or sorption/retardation<br>(for uncontaminated<br>sediments) of key<br>contaminants of<br>concern. | Qafoku et al. 2005. The<br>basic experimental data<br>that is in the form of<br>chemical concentration as<br>a function of leaching<br>volume of fluid, must be<br>modeled with various<br>commercial and research<br>codes to yield useable<br>information. CXTFIT is<br>used to fit physical<br>transport parameters such<br>as the dispersivity, while<br>other models are linked<br>with a solver of the<br>advective-dispersion<br>equation to describe<br>1-dimensional reactive<br>transport models include<br>a commercial one (the<br>Geochemists Workbench)<br>and others assembled by<br>the research team<br>including the Distributed<br>Rate Model (DRM) and<br>the Dual Continuum<br>Model (DCM). These are<br>described below. | Kinetic Desorption and<br>Sorption of U(VI) During<br>Reactive Transport in a<br>Contaminated Hanford<br>Sediment              |
| MINTEQA2 Version 4    | Commercial software<br>used to calculate<br>aqueous speciation,<br>precipitation/dissolution,<br>and adsorption/<br>desorption equilibria for<br>low to intermediate-<br>strength solutions.   | Code published by<br>Allison et al. 1991 and<br>1998 linked to a<br>thermodynamic database<br>of our own synthesis (see<br>below).   |  |
| Geochemists Workbench | Commercial software to<br>calculate geochemical<br>equilibria, reaction<br>network modeling, and<br>reactive transport.  | Geochemists Workbench<br>Release 6 from Craig<br>Bethke, Hydrogeology<br>Program, University of<br>Illinois.   |  |
| CXTFIT                | Commercial software<br>for fitting column<br>effluent data.  | Toride et al. 1999   | The CXTFIT Code for<br>Estimating Transport<br>Parameters from Laboratory<br>or Field Tracer Experiments                       |
| FITEQL (V 4.0)        | Commercial software<br>used to calculate<br>equilibrium constants<br>and their statistics for<br>aqueous, surface and<br>precipitated phases from<br>batch experimental data.  | Herbelin and Westall<br>1999   | FITEQL: A Computer<br>Program for Determination of<br>Chemical Equilibrium<br>Constants from Experimental<br>Data, Version 4.0 |

| Method   | Analysis  | Document Number                                      | Procedure/Document Title  |
|--|---|--|---|
| GMIN   | An equilibrium<br>geochemical model used<br>to calculate aqueous<br>speciation, precipitation/<br>dissolution, and<br>adsorption desorption<br>equilibria for high ionic<br>strength solutions.<br>Maintained by PNNL.  | Felmy 1995   | GMIN. A Computerized<br>Chemical Equilibrium<br>Program Using a Constrained<br>Minimization of the Gibbs<br>Free Energy: Summary<br>Report  |
| Spectral Fitting Software                                      | Commercial software<br>used to fit fluorescence<br>emission spectra on<br>U(VI) derived from<br>CLIFS analyses. The<br>fitting allows determina-<br>tion of the precise<br>spectral wavelengths<br>and deconvolutes<br>spectral signatures<br>resulting from multiple<br>fundamental species.   | Beechem et al. 1991                                  | Globals Unlimited   |
| Phase Identification for<br>Powder Diffraction<br>(JADE+, V 5) | Commercial software<br>used to manipulate<br>powder diffraction files<br>are for comparison with<br>reference spectra in for<br>mineral identification.   | Materials Data Inc.,<br>Livermore, CA; ICDD,<br>2003 | JCPDS Powder Diffraction<br>Files, PDF  |
| Reactive Transport<br>Modeling                                 | The Dual Continuum<br>Model (DCM) is used to<br>model the reactive<br>transport of contami-<br>nants 1-dimensional<br>laboratory columns and<br>in multidimensional<br>field simulations. The<br>model is a reaction-<br>based simulator and<br>requires significant<br>parameterization using<br>batch and column data,<br>and physical measure-<br>ments of sediment<br>characteristics.<br>Maintained by LANL. | Lichtner et al. 2000;<br>Lichtner et al. 2001        | Critique of Dual Continuum<br>Formulations of<br>Multicomponent Reactive<br>Transport in Fractured Porous<br>Media, Dynamics of Fluids in<br>Fractured Rock.<br>FLOTRAN: User's Manual. |
| Empirical Kinetic<br>Modeling                                  | The distributed rate<br>model (DRM) is used to<br>empirically describe<br>complex kinetic<br>desorption/dissolution<br>phenomena in sediment<br>that is controlled by<br>chemical kinetics or   | Culver et al. 1997                                   | Modeling the Desorption of<br>Organic Contaminants from<br>Long-Term Contaminated<br>Soil Using Distributed Mass<br>Transfer Rates  |

| diffuse mass transport.<br>The basic model<br>describes kinetic<br>phenomena using a<br>statistical distribution of<br>first order rate constants.  |   |   |
|---|---|---|
| Maintained at PNNL.   |   |   |
| The surface complex-<br>ation model (SCM) is<br>used to describe the<br>surface chemical<br>reactions of U(VI) that<br>are responsible for its<br>adsorption to vadose<br>zone and aquifer<br>sediments. Maintained<br>by USGS.   | Davis et al. 2004   | Approaches to Surface<br>Complexation Modeling of<br>Uranium(VI) Adsorption on<br>Aquifer Sediments   |
| A large thermodynamic<br>database is maintained<br>and constantly updated<br>based on literature<br>advances. The database<br>describes stability con-<br>stants for aqueous<br>complexes and solubil-<br>ity products for precip-<br>itated phases relevant to<br>S&T research and<br>issues. This database is<br>used in almost every<br>S&T geochemical study.<br>There are many hun-<br>dreds of entries in the<br>database for a variety of<br>contaminants that is<br>used in MINTEQA@;<br>Geochemists Work-<br>bench, and all of the<br>reactive transport codes.<br>Maintained at PNNL. | The database relies on the<br>following and many other<br>sources: Grenthe et al.<br>1992 (U); Guillaumount<br>et al. 2003 (U); Rard<br>1999 (Tc).  |   |
| ausraazst-zcatacsciisiusjootuotr  | ation model (SCM) is<br>issed to describe the<br>purface chemical<br>eactions of U(VI) that<br>are responsible for its<br>adsorption to vadose<br>cone and aquifer<br>rediments. Maintained<br>by USGS.<br>A large thermodynamic<br>latabase is maintained<br>and constantly updated<br>based on literature<br>advances. The database<br>describes stability con-<br>itants for aqueous<br>complexes and solubil-<br>ty products for precip-<br>tated phases relevant to<br>S&T research and<br>ssues. This database is<br>used in almost every<br>S&T geochemical study.<br>There are many hun-<br>treds of entries in the<br>latabase for a variety of<br>contaminants that is<br>used in MINTEQA@;<br>Geochemists Work-<br>bench, and all of the<br>eactive transport codes. | tion model (SCM) is<br>issed to describe the<br>purface chemical<br>eactions of U(VI) that<br>ire responsible for its<br>idsorption to vadose<br>cone and aquifer<br>rediments. Maintained<br>by USGS.<br>A large thermodynamic<br>latabase is maintained<br>ind constantly updated<br>ased on literature<br>idvances. The database<br>lescribes stability con-<br>itants for aqueous<br>complexes and solubil-<br>ty products for precip-<br>tated phases relevant to<br>S&T research and<br>ssues. This database is<br>ised in almost every<br>S&T geochemical study.<br>There are many hun-<br>freds of entries in the<br>latabase for a variety of<br>contaminants that is<br>ised in MINTEQA@;<br>Geochemists Work-<br>pench, and all of the<br>eactive transport codes. |

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Appendix C Experimental and Modeling Procedures Development for the Rifle IFC Site Project

# Appendix C Experimental and Modeling Procedures Development for the Rifle IFC Site Project

## **C.1 Introduction**

Laboratory activities shall be directed and controlled by internally approved procedures using techniques appropriate for the identified purpose. Many recognized, well-established methods and procedures already exist that may be incorporated into technical procedures to meet the client needs (e.g., consensus methods). However, because complex matrices usually require variation from published procedures, a flexible approach must be available to allow development, modification, and enhancement of a procedure on a real-time basis. This section describes the basic requirements for the development, qualification, change control, and routine review of procedures.

## C.2 Procedure Development

Step 1. If a procedure exists that meets the project needs, no procedure development is required.

If a procedure does not exist that meets the project needs, develop a test plan that documents the approach.

**Step 2.** Ensure that the requirements in the SBMS subject area (<u>http://sbms.pnl.gov/standard/74/7400t010.htm</u>) are met for PNNL procedures and test plans.

Step 3. Include the following in all procedures and test plans:

- Pagination Each page of the document must show the unique identifier and revision number as a minimum.
- Effective Date The date on which all work utilizing the document shall be implemented according to the document.
- Title The title of the document must be:
  - concise, clear, and descriptive of the system, equipment, process, or activity
  - applicable to the procedure and activity
  - unique to assist the user in identifying the correct procedure.
- Quality Control and Method Performance Technical procedures must include or reference the acceptance and performance criteria for precision, accuracy, calibration, and detection limit (as appropriate) established during the qualification experiments (e.g., references to the performance criteria in this plan, or specify client required criteria if different). Test plans must include the

expected acceptance and performance criteria for precision, accuracy, calibration, and detection limit (as appropriate). Qualification data shall be traceable to the procedure it supports.

- Use Category All analytical procedures and test plans must be designated as Mandatory Use or Reference Use.
- Reference Documents State the references used to develop the procedure or test plan. Include the following:
  - title
  - authors
  - year published
  - publisher.
- Document Code
- Revision.

**Step 4**. If a published, well-established method (e.g., American Society for Testing and Materials, EPA) already exists and is to be used, complete one of the following actions:

- Rewrite the procedure in PNNL format and language, making the procedure specific to the laboratory's or contractor institution's operations. Qualify the procedure prior to use.
- Provide a cover page, in PNNL or equivalent format, which includes the required elements in steps 2 and 3 above. In the Work Instruction section, include a reference to the attached published method. Any exceptions to the attached method are stated in the Work Instruction section. Qualify prior to use.
- Provide a cover page, in PNNL format, that includes the required elements from steps 2 and 3 above. In the Work Instructions section, include a reference to the attached published method. Any exceptions to the attached method are stated in the Work Instructions section. Qualification is performed during use (i.e., test plan).

Step 5. The client shall agree on the procedures/test plans used according to one of the following:

- Through the work authorizing document (procedures and/or test plans)
- Through the work authorizing document and the opportunity for review and acceptance of the procedures and/or test plans developed as part of the scope of work.

## C.3 Procedure Qualification

Technical procedures used for the first time in the laboratory must be qualified before reporting results to any client. Technical procedures are qualified during work execution. Qualification includes the selection of appropriate quality control checks to permit the evaluation of data quality and includes the following steps.

Step 1. Determine the need for qualification:

- single project use (e.g., test plan)
- long-term use (e.g., procedure or eventual procedure)

Determine what test materials will be used to conduct the qualification:

- reference materials (e.g., National Standards and Technology)
- simulants (e.g., internally prepared)
- sample spikes/duplicates (e.g., reference materials added to the sample matrix)
- combination of the above.

Determine how the qualification will be performed based on the data quality required by the project:

- use proposed method with identified test materials
- compare established method to proposed method
- use interlaboratory comparisons.

**Step 2**. Use a suitable number of replicate determinations to provide a measure of statistical control. Generally accepted standards dictate using a minimum of four replicates for each test case. Whenever possible, seven replicates should be used. These data are used to establish statistical control on an advisory basis until sufficient data are acquired, typically considered to be 30 data sets.

**Step 3.** Evaluate the procedure/test plan for its overall effectiveness in the areas of sensitivity, (method detection level) selectivity, linear range limitations, matrix or analytical precision and accuracy and counting statistics (minimum detectable activity and counter performance for radiochemistry), as applicable to the technique and/or analyte and depending on whether the technique is preparative, analytical, or encompasses both. This requires that testing include blank evaluation, precision and accuracy determination, efficiency, uncertainty, and determination of interferences as appropriate to the technique (i.e., preparative versus determinative).

**Step 4**. Make all qualification data traceable to the technical procedures(s) or test plan(s) it supports and retain it on file to enable retrospective examination should the need arise.

## C.4 Procedure Change Control

No technical procedure can be expected to be applicable, as written, to every type of sample the laboratory may receive. The primary concern when deviating from or changing a procedure must be whether or not the change has a negative impact on the client's data quality requirements. The following describes the types of changes, which may occur during work execution and the specific action required.

**Immediate Actions:** If personnel hazard or equipment damage is imminent, take immediate action to make the situation safe, as described below:

- The procedure user has the authority to immediately deviate from or curtail the use of the procedure and to secure processes, equipment, or systems as necessary to mitigate the situation. The user shall notify other impacted workers.
- The line manager must be informed of the situation as soon as reasonably possible.
- The Project Manager should be informed of the situation as soon as reasonably possible.

- The Project Manager should evaluate the situation to determine any impacts on the project, similar procedures, processes, equipment, or systems.
- The Project Manager directs the revision of the procedure as described in the Procedure Development process above if the problem was procedure based. **Note:** See also the SBMS subject area, "<u>Stopping and Restarting Work (Safety Rights and Responsibility)</u>."

**Substitutions:** Project staff make an adjustment in a procedure that a reasonable, technically competent person would be expected to consider equivalent. The substitution must have no significant effect on the final analytical results (e.g., substituting a different column with equivalent performance characteristics, using glassware other than that specified when it has no effect on analytical processes) and must not change the existing environmental, safety and health conditions.

Because substitution does not impact the method performed or the final analytical data, no documentation of change is required other than that necessary to allow reproduction of results.

**Deviations:** Deviation is divergence from the original procedure that does not adversely impact the analyst's ability to meet the precision, accuracy, detection limit, selectivity, and quality control criteria of the procedure (e.g., use of packed versus capillary columns). Therefore, the decision to deviate shall be based on published literature (e.g., alternate methods) and/or known sample chemistry.

Deviation requires documenting the changes made to a procedure. Documentation of deviations made shall be included in the final report narrative. Justification of the deviation should be evident in the acceptable performance associated with the final results and should also be discussed. Acceptable performance shall be demonstrated by the analyst's ability to meet or exceed the original method's precision, accuracy, detection limit, selectivity, and quality control criteria. When a deviation is used routinely, it shall be incorporated into the procedure.

- **Pre-Planned Deviations:** Pre-Planned deviations are those changes that are known before a procedure is applied. In this case the deviation(s) shall be documented, approval of the Project Manager shall be obtained, and the Project Manager shall notify the client for acceptance prior to sample analysis. The deviation shall be documented in the project record, and summarized in the final report to the client. A test plan may be used to document the deviation to the procedure. The notification and acceptance may be by an electronic mail message, DSI, memo or other written documentation.
- **Real-Time Deviations:** Real-time deviations are those changes that become necessary during the application of a procedure. As long as the deviation does not negatively impact the client's data quality requirements, an explanation in the final report is sufficient documentation. Also, the client shall be notified as soon as possible after the deviation occurs. Project staff are responsible for ensuring client notification.

**Modifications:** Modification changes the character of a procedure, and thereby potentially limits a procedure's ability to meet the originally stated precision, accuracy, detection limit, selectivity, and quality control criteria (e.g., microwave versus beaker digestion). Because the impact of such a modification cannot be ascertained before implementation, it must be demonstrated by application. Modifications shall not be performed during real-time project work activities.

Modification requires the procedure to be qualified, documented, approved, and agreed upon with the client before work. Justification of the modification should be evident in the quality control data associated with the final results and should also be discussed. A modification with long-term applicability should be developed into a new procedure that is issued with a new title and code.

**Note:** Method modification is not permitted when a regulatory method must be used for client work due to regulation. The only exception to this rule is when DOE OBER and DOE LM have first been notified and has approved use of the modified method. Method qualification is required prior to approval.

**Interim Change Notices:** Project staff use the Interim Change Notice (ICN) Form for the purpose of making an editorial correction or simple change to a document. The ICN provides for identifying, approving, and issuing the change within a short period of time. The ICN receives the same level of review and approval as the original document if the change is technical in nature. Since multiple ICNs can make a document difficult to implement, it is policy that a document be revised when a change is extensive or there are already three ICNs applied to the document. **Note:** ICNs shall not be used for modifications.

# C.5 Routine Review of Procedures

The Project Manager ensures that:

- Procedures to support the project have been reviewed at least every 24 months to ensure that they are still accurate. See Section C.6, "Suggested Guidelines" for examples of review activities that could occur.
- Documentation of this review has been provided in a memo or electronic mail message summarizing the conclusions of the review.
- Reviewed documentation is in the project records.

# C.6 Suggested Guidelines

The following are examples of procedure review activities that could occur:

- Review the procedure and the source requirements to determine if they are still accurate.
- Determine if any new hazards have been introduced.
- Evaluate procedure deviations at this time to determine if procedure revision is warranted.
- Determine if any facility modifications have been made that could affect the performance of the work or equipment.
- Review internal or external (e.g., regulatory or client) requirements to determine if any have changed.
- Review the number and type of interim changes that have been made to the procedure (see the Document Control section).

The review process may result in revising the procedure, or issuing an interim change notice to the procedure. If a revision or interim change notice is required, then follow the requirements in this section or the Document Control section.

## C.7 References

PNNL. 2004. "<u>Procedures, Permits, and Other Work Instructions</u>." Standards-Based Management System, Pacific Northwest National Laboratory, Richland, Washington. Available online at <u>http://sbms.pnl.gov/standard/74/7400t010.htm</u>.

PNNL. 2006. "Stopping and Restarting Work (Safety Rights and Responsibility)." Standards-Based Management System, Pacific Northwest National Laboratory, Richland, Washington. Available online at <a href="http://sbms.pnl.gov/standard/0m/0m00t010.htm">http://sbms.pnl.gov/standard/0m/0m00t010.htm</a>.

Appendix D Detailed Rifle IFC Project Schedule

# Appendix D Detailed Rifle IFC Project Schedule

|    |  | Start   | Finish  |         | 2007     |          |       |     |      |      |        |           |         |
|----|--|---------|---------|---------|----------|----------|-------|-----|------|------|--------|-----------|---------|
|    | Activity Name  | Date    | Date    | January | February | March    | April | May | June | July | August | September | October |
| 1  | Draft Rifle IFC PMP  | 1/2/07  | 1/15/07 | Ì       |          |          |       |     |      |      |        |           |         |
| 2  | Revise Rifle IFC PMP   | 5/7/07  | 5/8/07  |         |          |          |       | *   |      |      |        |           |         |
| 3  | Rifle IFC Planning Meeting<br>Grand Junction, CO                   | 2/27/07 | 3/1/07  |         | 4        |          |       |     |      |      |        |           |         |
| 4  | Preparation for Planning<br>Meeting                                | 2/1/07  | 2/23/07 | 4       | ļ        |          |       |     |      |      |        |           |         |
| 5  | Rifle IFC PNNL<br>Review/Kickoff Meeting                           | 5/10/07 |         |         |          |          |       | •   |      |      |        |           |         |
| 6  | Revise project documents<br>per PNNL Review/kickoff<br>Meeting     | 5/11/07 | 5/18/07 |         |          |          |       | *   |      |      |        |           |         |
| 7  | Develop subcontract<br>language for Co-PI's                        | 1/29/07 | 3/30/07 | 0       |          |          | >     |     |      |      |        |           |         |
| 8  | Process subcontracts   | 3/19/07 | 4/30/07 |         |          | <u> </u> |       | Ŷ   |      |      |        |           |         |
| 9  | Develop detailed project<br>schedule                               | 5/7/07  | 5/10/07 |         |          |          |       | 4   |      |      |        |           |         |
| 10 | Develop Overall Health and<br>Safety Plan                          | 5/8/07  | 5/9/07  |         |          |          |       | 0   |      |      |        |           |         |
| 11 | Develop backhoe sampling<br>plan                                   | 5/8/07  | 5/10/07 |         |          |          |       | *   |      |      |        |           |         |
| 12 | Develop Field Site<br>Management Plan                              | 5/9/07  | 5/15/07 |         |          |          |       |     |      |      |        |           |         |
| 13 | Conduct backhoe sampling<br>for experimental site<br>investigation | 5/16/07 | 5/17/07 |         |          |          |       | \$  |      |      |        |           |         |
| 14 | Develop Experimental Plan<br>for 2007 field experiment             | 5/11/07 | 5/18/07 |         |          |          |       | *   |      |      |        |           |         |
| 15 | Co-PI review of<br>Experimental Plan for 2007<br>field experiment  | 5/21/07 | 5/25/07 |         |          |          |       | ×   |      |      |        |           |         |
|    |  |         |         | January | February | March    | April | Мау | June | July | August | September | October |

|    |   | Start   | Finish  |         |          |       |       | 20  | 07   |      |        |           |         |
|----|---|---------|---------|---------|----------|-------|-------|-----|------|------|--------|-----------|---------|
|    | Activity Name   | Date    | Date    | January | February | March | April | May | June | July | August | September | October |
| 16 | ERSP Field Advisory Team<br>review of Experimental Plan<br>for 2007 Field Experiment<br>and Overall FY-07 Plan  | 5/29/07 | 6/8/07  |         |          |       |       |     | Ì    |      |        |           |         |
| 17 | Incorporate Review<br>Comments  | 6/11/07 | 6/14/07 |         |          |       |       |     | ζφ.  |      |        |           |         |
| 18 | Obtain backhoe samples<br>for initial column<br>experiments for protein<br>expression   | 1/16/07 | 1/18/07 | Ø       |          |       |       |     |      |      |        |           |         |
| 19 | Conduct initial column<br>experiments at UCB  | 2/5/07  | 6/1/07  |         | Ň.       |       |       |     |      |      |        |           |         |
| 20 | Develop summary of FY-07<br>Plan  | 3/5/07  | 5/25/07 | )       |          | ¥     |       |     |      |      |        |           |         |
| 21 | Planning for backhoe<br>sampling and well point<br>installations  | 4/30/07 | 5/15/07 |         |          |       | <     |     |      |      |        |           |         |
| 22 | Collect backhoe samples<br>and install well points to<br>constrain locations for F-0<br>and subsequent field<br>experiments                                       | 5/16/07 | 5/18/07 |         |          |       |       | Ø.  |      |      |        |           |         |
| 23 | Analyze groundwater and<br>sediment samples from<br>backhoe and well points to<br>confirm locations of<br>experimental plots and<br>provide initial sorption data | 5/21/07 | 7/30/07 |         |          |       |       |     |      |      | ]      |           |         |
| 24 | Well installation for 2007<br>field experiment  | 6/18/07 | 6/27/07 |         |          |       |       |     |      |      |        |           |         |
| 25 | Conduct EM-31 Survey of<br>Flood Plain  | 6/11/07 | 6/13/07 |         |          |       |       |     | ۵×   |      |        |           |         |
| 26 | Initial Set up of field site<br>infrastructure  | 4/27/07 | 7/2/07  |         |          |       | 0     |     |      | Ŷ    |        |           |         |
| 27 | Well development and set<br>up  | 7/3/07  | 7/16/07 |         |          |       |       |     |      | ×.   |        |           |         |
|    |   |         |         | January | February | March | April | May | June | July | August | September | October |

|    | Activity Name  | Start   | Finish   |         |          |       |              | 20  | 07          |      |        |           |          |
|----|--|---------|----------|---------|----------|-------|--------------|-----|-------------|------|--------|-----------|----------|
|    | Activity Name  | Date    | Date     | January | February | March | April        | May | June        | July | August | September | October  |
| 28 | Conduct slug tests and flow<br>meter tests   | 7/16/07 | 7/27/07  |         |          | /     |              |     |             | - 🍋  |        |           |          |
| 29 | Perform GPS location for<br>new experimental plot wells  | 7/30/07 | 7/31/07  |         |          | ,     | \            |     |             | 8    | X      |           |          |
| 30 | Install multiparameter<br>probes and pressure<br>transducers   | 7/28/07 | 8/8/07   |         |          |       | $\backslash$ |     |             |      |        |           |          |
| 31 | Conduct surface and<br>borehole geophysics   | 7/28/07 | 8/3/07   |         |          |       |              |     |             | Å    |        |           |          |
| 32 | Mix Tank with acetate and<br>Br  | 8/5/07  | 8/7/07   |         |          |       |              |     |             |      | Ŷ      |           |          |
| 33 | Start acetate and Br<br>injection for 2007<br>Experiemnt (F-0)   | 8/8/07  |          |         |          |       |              |     |             |      | ¥      |           |          |
| 34 | Conduct geochemical,<br>dissolved gas, genomic and<br>proteomic sampling per<br>2007 Experimental Plan | 7/30/07 | 9/28/07  |         |          |       | )            |     |             | ×.   |        |           |          |
| 35 | Acetate and Br injection   | 8/8/07  | 8/17/07  |         |          |       |              |     |             |      |        |           |          |
| 36 | Groundwater flush  | 8/19/07 | 8/24/07  |         |          |       |              |     |             |      | - X    |           |          |
| 37 | Restart Acetate and Br<br>injection  | 8/25/07 | 9/15/07  |         |          |       |              |     |             |      | l 4    |           |          |
| 38 | Preparation for drilling and<br>well installation (F-0 and for<br>sorption experiments)                | 9/4/07  | 10/4/07  |         |          |       |              |     |             |      |        |           | <u> </u> |
| 39 | Drilling and well installation   | 10/8/07 | 10/10/07 |         |          |       |              | /   |             |      |        |           | 0        |
| 40 | Backhoe sample<br>preparation  | 8/13/07 | 8/16/07  |         |          |       |              |     | $\setminus$ |      | ~~~~/  |           |          |
| 41 | Background and sorption<br>experiment backhoe<br>samples   | 8/17/07 | 8/18/07  |         |          |       |              |     |             |      | ∛      |           |          |
|    |  |         |          | January | February | March | April        | May | June        | July | August | September | October  |

|    | Activity Name   | Start   | Finish  |         | 2007     |       |       |     |      |      |        |           |         |
|----|---|---------|---------|---------|----------|-------|-------|-----|------|------|--------|-----------|---------|
|    | Activity Name   | Date    | Date    | January | February | March | April | May | June | July | August | September | October |
| 42 | Perform baseline<br>mineralogical analyses on<br>sediments obtained from<br>F-0 experimental plot | 7/9/07  | 9/28/07 |         |          |       |       |     |      | *    |        | •         |         |
| 43 | Perform initial<br>microbiological sampling for<br>natural bioreduction                           | 7/29/07 | 8/3/07  |         |          |       |       |     |      | ð    | Þ      |           |         |
|    | Conduct Fe-57 U<br>bioreduction column<br>experiments (Princeton)                                 | 7/2/07  | 9/10/07 |         |          |       |       |     |      |      |        | V         |         |
| 45 | write and submit abstracts<br>to GSA and Fall AGU   | 7/2/07  | 9/6/07  |         |          |       |       |     |      |      |        | <b> </b>  |         |
|    |   |         |         | January | February | March | April | May | June | July | August | September | October |

# Appendix E ERSD Management Plan for the Integrated Field Challenge Projects

# Appendix E ERSD Management Plan for the Integrated Field Challenge Projects

Environmental Remediation Sciences Division Office of Biological and Environmental Research

September 2007

# ERSD Management Plan for the Integrated Field Challenge (IFC) Projects

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## Introduction

In the fall of 2006, the Environmental Remediation Sciences Division (ERSD), within the Office of Biological and Environmental Research, established three Integrated Field-Challenge (IFC) projects. The IFC projects, which are listed below, are each funded at approximately \$3 million per year over five years. The purpose of the IFCs is to enable multi-disciplinary research teams to perform integrated and comprehensive studies of key physical, chemical and biological processes that control the fate and transport of subsurface contaminants at DOE sites. The IFCs are intended to serve as central foci for the broader research activities within the ERSD program. The IFCs should also serve as valuable resources for investigators within ERSD to obtain natural materials for use in laboratory investigations and to formulate independent research projects that are motivated by the observations that are made at the IFCs. To this end, an important function of the IFCs is to become a community resource where the unique and extensive data sets collected at these sites are archived and made readily available to the wider ERSD and scientific communities.

#### Oak Ridge IFC

Location: Y-12 Site on the Oak Ridge Reservation, Oak Ridge, TN Principal Investigator: Dr. Phil Jardine, Oak Ridge National Laboratory (ORNL) Field Site Manager: Mr. Dave Watson, ORNL Further information about the Oak Ridge IFC will soon be available on the web.

#### Hanford 300-Area IFC

Location: 300 Area of the Hanford Site, Richland, WA Principal Investigator: Dr. John Zachara, Pacific Northwest National Laboratory (PNNL) Field Site Manager: Mr. Mark Freshley, PNNL Further information about the Hanford 300 IFC will soon be available on the web.

#### Old Rifle IFC

Location: Old Rifle Uranium Mill Tailings Remedial Action (UMTRA) Site, Rifle, CO Principal Investigator: Dr. Phil Long, PNNL Field Site Manager: Mr. Dick Dayvault, S.M. Stoller Corporation, Inc. Further information about the Old Rifle IFC will soon be available on the web.

## **Documentation of IFC Management and Operations**

Each IFC is expected to develop and post on their web site a set of IFC management and operations documents that will help to govern IFC activities. As outlined in DOE's 2006 IFC solicitation, these management and operations documents are expected to include:

- Management Plan for all project (including field site) activities,
- Overall Health and Safety Plan (HASP) tiered from the DOE host site HASP,
- Quality Assurance/Quality Control (QA/QC) Plan,
- Communications/Community Interactions Plan, and
- Field Site Closure Outline.

The Communications/Community Interactions Plan and the Field Site Closure Outline could be included as separate sections within the overall Management Plan.

Each IFC also should develop a data management approach that addresses the needs of IFC team members as well as non-team members interested in making use of the IFC field site or research results. The expected content for these plans is outlined in DOE's 2006 IFC solicitation.

Additional management and operational documents may be developed and posted by each IFC as needed.

## **Quarterly Communications and Reporting**

The Field Site Manager and the PI for each IFC are expected to participate in a quarterly teleconference for all three IFCs. The purpose of having one teleconference call with all three IFCs and ERSD program managers present is to ensure cross fertilization of lessons learned and enable coordination with ERSD program managers. These quarterly teleconference calls are expected to occur in October, January, and July each year. Instead of holding a quarterly teleconference call in April each year, the IFCs are expected to participate in a face to face meeting with the ERSD program managers at the time of the annual ERSD PI meeting.

Prior to each quarterly teleconference call, each IFC is expected to submit to their appropriate ERSD program manager a written quarterly report. The quarterly reports will be due to ERSD by the seventh of October, January, April, and July each year. The quarterly report should include the following sections:

Overview & Highlights - speaking engagements, important publications, press releases, etc.

Significant Changes - in scope, experimental design or staffing,

Management & Operations – updates to documentation that is posted on the IFC web site, subcontracting updates, team meeting summaries, etc.,

Quarterly Research Highlights - highlights from each task,

Non-IFC Project Activities – a list of non-IFC PI queries and subject(s), number and type of samples and identity of organizations that received samples from the IFC field site, including on-site use by non-IFC PI's, and concerns/challenges/opportunities with non-IFC PI's that are outside of agreed upon plans,

Funding Issues – funding received to date from ERSD, funding spent in the quarter, and funding remaining for the FY,

Upcoming Plans/Issues – research plans (especially field activities) for the next quarter and other issues as needed, and

Peer Reviewed Publications, Abstracts, and Presentations - citations.

## **Annual Reports**

Each IFC is expected to prepare an Annual Report to summarize the overall status of the project, highlight the important results from the previous year and present research plans for the upcoming year. The IFC Annual Reports should be submitted to the ERSD by February 15<sup>th</sup> each year. This will give ERSD staff and the Field Research Executive Committee, whose roles and responsibilities are described in the next section, sufficient time to review the reports and provide feedback to the IFC PIs before the Annual ERSP PIs Meeting each spring. In addition to the IFC Annual Reports, the PI's are expected to submit Field Work Proposals (FWPs) each year, which are required for budgetary purposes.

The IFC Annual Reports are expected to have the following format:

#### **Cover Page**

Project Title: Reporting Period: PI: Co-PIs and their overall responsibilities and funding levels.

#### **Project Status: A Five Year Perspective**

Update the five-year Milestone Chart (Timeline) that was included in the original IFC proposal. Use the following color code to indicate which tasks are complete (blue), in progress (yellow), and remain to be started (red).

Progress in key areas of the originally proposed hypotheses should be discussed. If the hypotheses have been modified over the last year please indicate these changes and explain the reasoning for the changes.

#### Major Accomplishments: Last 12 Months

Briefly summarize how the research goals from the previous year have been met.

#### **Research Plans: Next 12 Months**

Briefly outline the main activities of the research for the upcoming year. This can be done in a task outline format but should describe how the upcoming tasks are related to the project hypotheses.

#### **Outreach Activities**

Samples that have been provided to investigators, external (non-IFC) PI's who have used the site, significant activities with EM, LM, site contractors, the public, meetings, news releases etc.

#### Challenges/Opportunities/Concerns

Discuss any challenges/opportunities/concerns, including new research that conflicts either physically or financially with the original goals/plans.

## Field Research Executive Committee: Role and Responsibilities

The primary role of the Field Research Executive Committee (FREC) is to provide ERSD with technical support and oversight for the management of the ERSD field research programs. The FREC is composed of the following scientists who provide a broad range of expertise in subsurface science:

Richelle Allen-King, University of New York at Buffalo

Roger Beckie, University of British Columbia

Susan Clark, Washington State University

Fred Day-Lewis, U.S. Geological Survey, Storrs, CT

Richard Deveraux, U.S. Environmental Protection Agency, Gulf Breeze, FL

Gordon Southam, University of Western Ontario

The FREC members will review the IFC Annual Reports and provide technical feedback to ERSD Program Managers and the IFC PIs. The FREC members also will be invited to attend the Annual ERSP PI Meetings. The IFC PIs should respond to the FREC members review comments before the Annual Meeting.

To enable FREC members to gain a more intimate knowledge of the IFC projects, ERSD will arrange for at least two members of the FREC to visit each of the IFC sites. Dates for the site visits will be arranged by the ERSD staff to accommodate the schedules of the FREC members and the IFC PIs.

# Appendix A: FY 2007 Research Update

ERSD plans to organize a teleconference (online presentation) for the IFC leads to update ERSD staff and the Field Research Executive Committee (FREC) on the research activities that have been initiated at the IFCs during the summer of FY 2007. This online meeting is expected to occur during late October early November 2007; the exact date and time will be decided in consultation with the IFC leads and the FREC members.

In these updates, the PIs are expected to summarize the major comments of the proposal reviewers and explain how these comments have been addressed in the experiments/activities undertaken during the summer of 2007, or will be addressed in future research/work. If any of the hypotheses for the project have been modified, these changes should be indicated and explained during the teleconference. These presentations should be about 45 minutes for each IFC, followed by 30 minutes of questions and discussion.

For the Oak Ridge IFC, ERSD required that a FY 2007 Implementation Plan for the IFC be prepared by the end of the second quarter of the fiscal year, in accordance with one of the quarterly milestones for the Performance Assessment Rating Tool (PART)

(<u>http://www.science.doe.gov/ober/performance.html#joule</u>). The Oak Ridge IFC Implementation Plan has been posted to a publicly available web site

(http://www.lbl.gov/ERSP/generalinfo/milestones/pdfs/Implement\_plan\_3\_29\_07.pdf). For the fourth quarter FY 2007 milestone, ERSD requires that a progress report for the Oak Ridge IFC Implementation Plan be prepared. ERSD expects that this progress report will include an outline and explanation of the summer 2007 experimental activities and how they address the hypotheses posed in the original proposal, as well as how the reviewer comments on the original proposal have been addressed. The PI for the Oak Ridge IFC should plan to provide the Implementation Plan progress report to participants on the October 2007 teleconference call.

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All Rifle IFC Project Participants (to be provided as a PDF).